



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:32 PM UTC

PDB ID : 7YFP / pdb_00007yfp
EMDB ID : EMD-33796
Title : The NuA4 histone acetyltransferase complex from *S. cerevisiae*
Authors : Ji, L.T.; Zhao, L.X.; Xu, K.; Gao, H.H.; Zhou, Y.; Kornberg, R.D.; Zhang, H.Q.
Deposited on : 2022-07-08
Resolution : 4.00 Å(reported)
Based on initial model : 5OJS

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

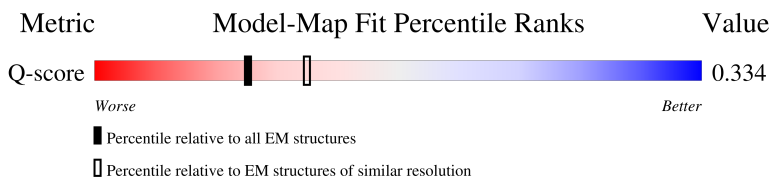
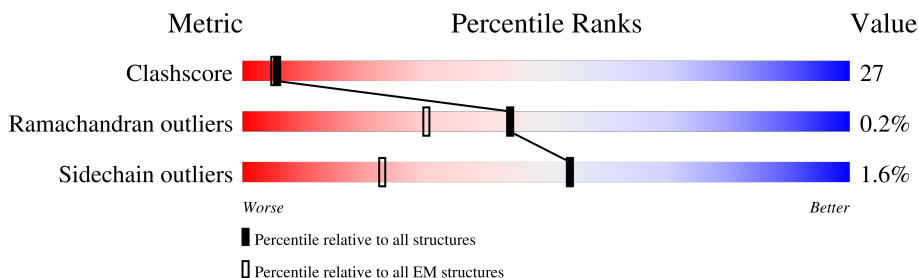
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	372	 6% 52% 48%
2	B	481	 47% 36% 16%
3	D	982	 27% 19% 54%
4	E	476	 26% 16% 58%

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Mol	Chain	Length	Quality of chain
5	F	832	 9% 6% 85%
6	T	3744	 21% 47% 44% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 40949 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total	C	N	O	S	0	0
			2904	1841	491	553	19		

- Molecule 2 is a protein called ARP4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	402	Total	C	N	O	S	0	0
			3172	2024	518	619	11		

- Molecule 3 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	454	Total	C	N	O	S	0	0
			3777	2392	683	691	11		

- Molecule 4 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	201	Total	C	N	O	S	0	0
			1668	1069	276	319	4		

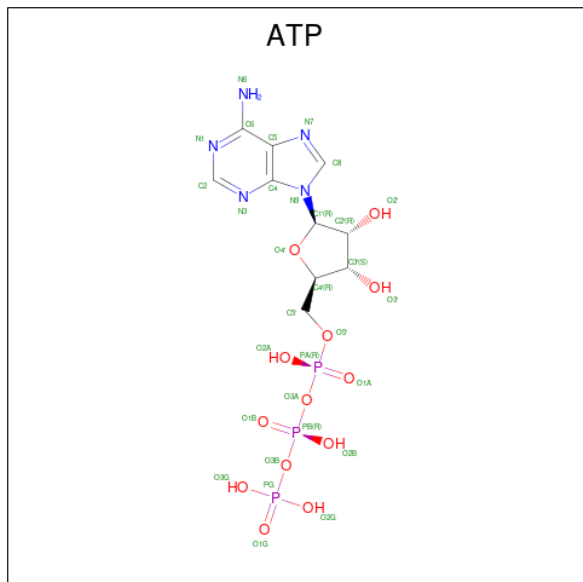
- Molecule 5 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	124	Total	C	N	O	S	0	0
			1023	653	177	190	3		

- Molecule 6 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	3475	Total	C	N	O	S	0	0
			28374	18368	4717	5169	120		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

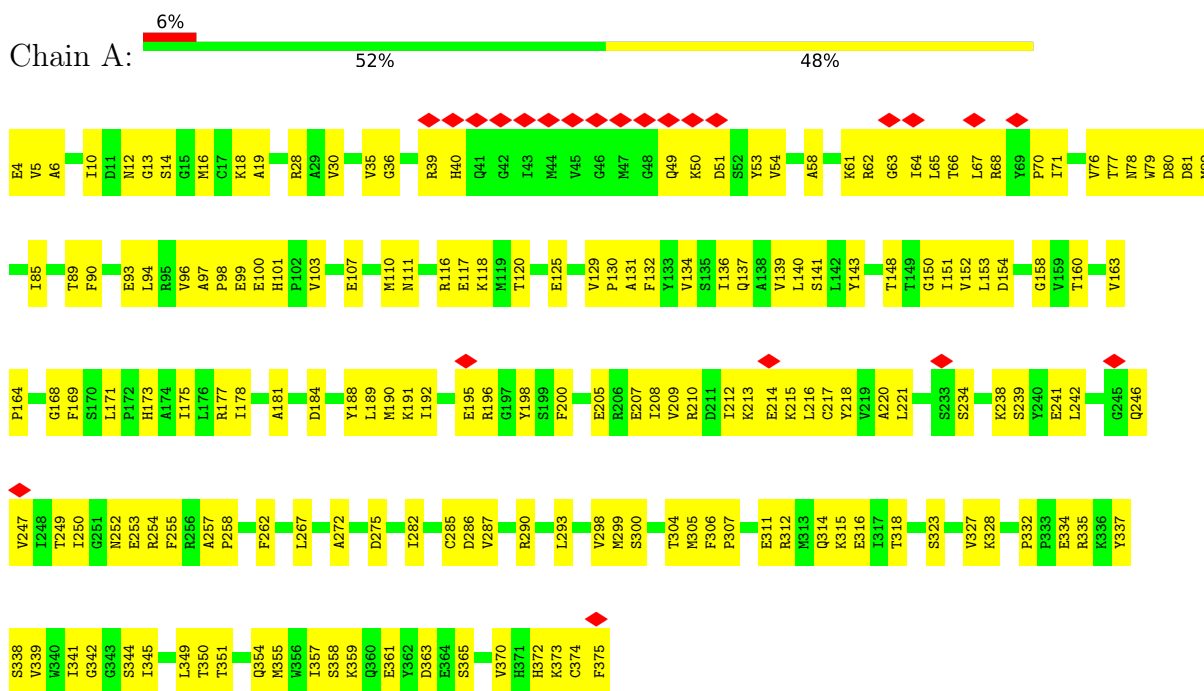


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	31	10	5	13	3	0

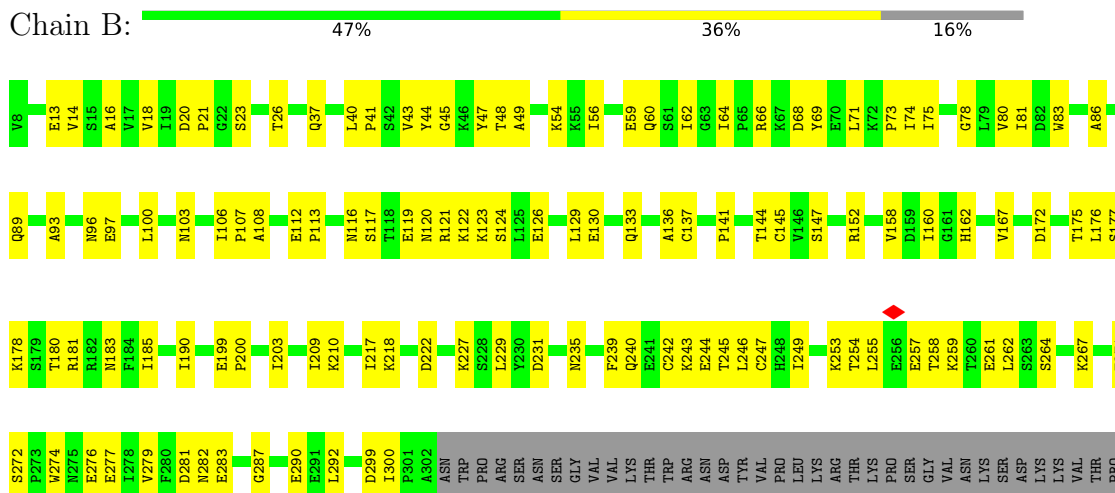
3 Residue-property plots

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



• Molecule 2: ARP4 isoform 1







S426	K496	E630	M691	I763	H837	D914	I1011	L1106	P1191	G1281	Q1350
L427	K497	V633	Q692	F766	L838	P915	I1011	L1107	E1192	V1284	I1351
A428	E498	V634	M693	K767	L839	I916	R1014	D1108	L1193	L1284	G1352
L429	E499	K635	D694	L768	Q840	I917	Y1018	H1109	L1198	L1285	N1353
T430	A500	D636	T697	S769	L842	E918	T1022	G1111	H1199	E1286	V1354
V431	E501	L637	F698	F770	N843	I921	T1022	L1112	D1203	L1289	I1357
Q432	E502	F638	F699	N771	Q844	D922	K1030	L1113	E1204	D1290	T1358
I433	K503	H639	M700	S772	N845	I922	S1031	Q1114	L1205	D1291	F1359
M434	L504	E640	I701	V773	L846	Q932	S1031	V1115	Y1206	V1292	C1360
K437	K504	C641	I702	N774	L847	Q933	P1036	N1116	T1207	C1294	L1361
L438	N505	I642	I705	L775	T648	P934	P1036	T1117	Y1207	E1295	S1362
L439	S506	I643	E705	F776	A849	Q935	Y1039	T1118	N1208	L1296	L1363
L440	S507	G644	L706	F777	R850	F936	T1040	R1123	K1209	L1297	T1366
M441	I507	L645	L707	N779	L851	F937	E1041	T1128	R1210	S1297	F1367
L442	Q508	K646	F708	I779	P852	P937	L1042	T1129	V1213	N1298	L1368
V443	D509	F647	Y709	N780	H853	S942	L1043	H1129	F1213	A1299	L1369
E444	N510	F648	Y710	E781	E854	H943	L1044	N1130	I1216	N1300	T1370
R445	D511	LYS	E711	V782	E855	N944	T1045	I1131	P1301	K1302	N1371
I446	K512	ASP	R712	L783	R856	V945	T1045	L1132	L1219	V1303	E1372
L447	D513	HIS	M713	L784	L857	R947	A1046	L1133	V1223	R1304	E1373
E452	E513	ASN	L714	L785	R858	I948	S1049	K1134	V1223	C1307	L1374
P458	S514	GLU	E715	P786	H859	L949	I1050	L1140	F1229	L1311	F1375
R459	E515	LEU	D716	H787	E860	G950	K1051	L1144	L1230	H1312	R1376
A460	E516	PRO	S717	L788	L861	K951	L1052	L1145	Q1234	I1313	L1377
K461	F517	THR	G718	N789	L862	L952	E1053	L1146	L1237	I1314	Q1379
L462	M518	GLU	L719	D790	E863	N956	R1054	L1155	L1237	S1315	E1380
L463	R519	LEU	L720	L792	P866	R957	I1057	Y1156	G1240	G1319	S1381
L464	K520	SER	Q724	L793	VAL	R957	E1058	I1157	G1240	I1320	L1382
M465	V521	PHE	L727	S795	LEU	P963	K1059	Y1158	V1245	V1323	V1383
I466	L522	ASP	T728	L796	ARG	T964	N1060	E1159	L1245	K1324	L1384
I467	GLU	K595	T729	L799	LEU	D965	F1061	P1158	T1248	L1325	A1385
I468	PRO	T596	E730	S799	VAL	L966	D1062	E1160	E1251	H1328	A1386
D469	ASP	I597	I731	T801	ALA	E967	T1066	E1161	A1252	S1329	A1387
S470	ASP	I598	L732	T802	PRO	E968	V1067	E1162	P1253	Q1330	E1388
Y471	ASP	H599	S733	A802	L805	D973	K1068	V1163	Q1075	F1332	D1389
M472	ASP	D600	G738	P805	L806	D979	R1070	V1163	D1071	L1333	E1390
R474	LEU	N605	L739	L807	P877	F980	R1071	I1171	Q1075	T1257	S1391
F475	LEU	N609	L740	L808	F878	K981	Q1075	Y1172	L1085	D1258	L1392
K476	PRO	E610	L741	Y808	L879	I982	S1085	K1174	V1086	S1259	S1393
T477	GLN	Y611	R742	R813	H890	N983	V1086	S1175	E1261	A1260	T1394
L478	PRO	T612	E743	R817	E896	G984	V1086	I1178	I1265	I1337	N1395
N479	LYS	T613	L744	R817	Q896	M985	V1086	Y1179	D1266	F1338	I1396
R480	LYS	V613	D678	R823	L896	P986	A1089	G1180	L1267	A1339	Q1397
Q481	GLU	A614	A679	R823	L876	E987	T1090	E1181	L1268	K1340	K1398
Y482	ASP	N615	R680	R826	P877	Q988	S1091	L1182	S1269	P1341	T1399
I485	ASN	P616	L682	N826	ASP	L1001	D1097	L1183	S1269	R1343	T1400
Y488	SER	K617	M683	L827	ASN	L1004	H1100	L1184	E1182	L1344	E1401
Y489	SER	L618	Y685	Y828	THR	Q1005	D1101	L1185	L1182	T1271	E1402
G490	ASP	L619	F756	Y828	THR	L1102	L1100	L1186	L1267	A1344	S1403
R491	VAL	M620	N757	T831	A910	S1006	L1102	L1187	L1268	L1345	T1404
Y492	GLU	S621	F688	R832	THR	Y1007	N1104	S1188	F1272	P1346	Q1407
E493	THR	V622	M689	P833	THR	Y1007	N1104	F1189	K1276	F1347	L1408
T494	GLU	R624	L762	L834	THR	Y1007	N1105	I1190	T1348	T1348	V1409
H495	ASP	V625	F626	S627	THR	Y1007	N1105	I1190	M1349	M1349	Q1410
	VAL	F627	Y628	E629	THR	Y1007	N1105	I1190			L1411
	VAL										





E3590	P3592	D3505	Q3406	P3305
M3691	V3596	M3506	Y3407	D3306
N3695	LYS	T3507	V3410	Y3307
	PRO	I3508	R3411	E3308
I3699	LEU	L3509	H3412	T3309
	LEU		S3413	
N3710	LYS	T3519	R3414	L3314
S3711	ASN		R3415	M3317
	HIS	V3522	E3416	
V3715	ASP	P3523	E3417	R3320
T3716	LEU	S3524	R3418	L3321
T3717	SER	N3525	M3419	E3322
	LEU		F3420	
I3720	PRO	K3528	Q3421	D3326
L3721		T3532	L3422	
	I3613	S3533	Y3423	K3331
I3724	F3614	L3534		E3332
	H3615		F3426	N3333
A3727		E3539	K3428	
V3728	V3620	D3540		V3336
S3729		F3541	S3431	
P3730	R3623	V3542	K3432	P3339
R3731	I3624	L3543	N3433	
N3732	T3625	P3544	V3434	N3343
L3733	P3626	R3545	E3435	
A3734	Q3629		T3436	
R3735	D3634	Q3551	R3437	K3348
T3736	S3635	Y3552	R3438	F3349
D3737	A3636	S3553	S3439	E3353
V3738	L3637	M3554	S3440	
N3739	E3638		I3441	Q3357
F3740	G3639	M3558	F3442	V3358
			F3443	
W3743	I3648	K3561	N3444	N3365
F3744		M3562	L3445	
		V3563	P3446	F3368
		I3564		I3369
		N3565	L3451	K3370
		N3566		I3371
		R3567	I3457	A3372
				R3373
		H3573	D3460	
		V3574		T3377
		D3575	F3464	V3378
			T3465	
		S3578	T3466	R3382
		G3579		G3383
		N3580	N3472	H3385
		V3581		
		F3582	K3476	I3393
		T3583		
		L3584	P3482	D3397
		E3585		G3398
		N3586	L3493	S3399
		L3587		V3400
		P3588	H3497	H3401
		Q3687	D3498	
		L3688	D3499	
		R3689		V3405

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0396	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/2968	0.36	0/4017
2	B	0.23	0/3241	0.38	0/4398
3	D	0.25	0/3859	0.48	0/5212
4	E	0.20	0/1707	0.38	0/2300
5	F	0.24	0/1046	0.55	0/1405
6	T	0.50	0/28991	0.72	4/39278 (0.0%)
All	All	0.44	0/41812	0.64	4/56610 (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
3	D	0	3
5	F	0	1
6	T	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	3592	PRO	N-CA-CB	6.65	110.23	103.25
6	T	1960	ALA	N-CA-C	-6.22	106.33	114.04
6	T	1436	ILE	N-CA-C	-5.66	107.36	112.12
6	T	2872	SER	N-CA-C	-5.47	107.25	114.04

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	535	SER	Peptide
3	D	540	ALA	Peptide
3	D	60	LYS	Peptide
5	F	560	VAL	Peptide
6	T	1366	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2904	0	2874	138	0
2	B	3172	0	3125	136	0
3	D	3777	0	3763	190	0
4	E	1668	0	1630	73	0
5	F	1023	0	999	58	0
6	T	28374	0	28736	1730	0
7	B	31	0	12	5	0
All	All	40949	0	41139	2238	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 27.

All (2238) 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)
6:T:480:ARG:HD3	6:T:1760:TYR:CD1	1.17	1.60
6:T:2320:LEU:CD1	6:T:2355:MET:HB3	1.26	1.58
6:T:480:ARG:CB	6:T:1760:TYR:CZ	1.86	1.55
6:T:480:ARG:HD3	6:T:1760:TYR:CE1	1.40	1.53
6:T:2320:LEU:HD11	6:T:2355:MET:C	1.30	1.50
6:T:2320:LEU:CD1	6:T:2355:MET:CB	1.85	1.50
6:T:694:ASP:CG	6:T:1585:ARG:HH11	1.15	1.45
6:T:2320:LEU:HD13	6:T:2355:MET:CB	1.42	1.44
6:T:1441:LEU:CD1	6:T:1473:LEU:HD13	1.51	1.41
6:T:1441:LEU:HD12	6:T:1473:LEU:CD1	1.49	1.40
6:T:560:MET:HA	6:T:1767:PHE:CZ	1.59	1.37
6:T:2325:LEU:CD2	6:T:2329:ARG:HA	1.53	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:HB3	6:T:1760:TYR:CZ	1.49	1.32
6:T:560:MET:HG2	6:T:1767:PHE:CE1	1.64	1.31
6:T:480:ARG:CD	6:T:1760:TYR:CE1	2.12	1.30
6:T:480:ARG:CD	6:T:1760:TYR:CD1	2.13	1.29
6:T:480:ARG:HB2	6:T:1760:TYR:CZ	1.52	1.28
6:T:2320:LEU:HD21	6:T:2358:SER:OG	1.33	1.27
6:T:2325:LEU:HD21	6:T:2329:ARG:CA	1.69	1.23
6:T:480:ARG:HB2	6:T:1760:TYR:CE1	1.74	1.21
6:T:480:ARG:HB3	6:T:1760:TYR:CE2	1.77	1.20
6:T:694:ASP:OD2	6:T:1585:ARG:NH1	1.73	1.19
6:T:560:MET:HG2	6:T:1767:PHE:CZ	1.76	1.19
6:T:2276:THR:CG2	6:T:2277:PRO:HD3	1.72	1.19
6:T:1594:THR:OG1	6:T:1595:PRO:HD3	1.40	1.18
6:T:694:ASP:CG	6:T:1585:ARG:NH1	2.00	1.16
6:T:629:GLU:CD	6:T:1717:GLN:HB3	1.69	1.16
6:T:2320:LEU:CD1	6:T:2355:MET:C	2.20	1.14
6:T:1441:LEU:CD1	6:T:1473:LEU:CD1	2.13	1.12
6:T:1441:LEU:HD12	6:T:1473:LEU:HD12	1.28	1.12
6:T:1441:LEU:HD13	6:T:1473:LEU:HD13	1.19	1.11
6:T:381:PHE:HB2	6:T:1858:ASP:OD1	1.50	1.10
6:T:480:ARG:CB	6:T:1760:TYR:CE1	2.32	1.09
6:T:480:ARG:CB	6:T:1760:TYR:OH	1.96	1.09
6:T:480:ARG:HB2	6:T:1760:TYR:OH	1.51	1.08
6:T:613:VAL:HG13	6:T:1536:ASP:OD1	1.53	1.07
6:T:1900:LEU:HD23	6:T:1900:LEU:H	1.17	1.06
6:T:1716:LEU:H	6:T:1716:LEU:HD12	1.16	1.05
6:T:1920:ILE:H	6:T:1920:ILE:HD12	1.21	1.05
6:T:1543:LEU:HD22	6:T:1543:LEU:H	1.20	1.05
6:T:1449:LEU:HD22	6:T:1484:PRO:HG2	1.35	1.04
6:T:611:TYR:CZ	6:T:1583:LYS:O	2.10	1.04
6:T:1441:LEU:HB2	6:T:1473:LEU:HD11	1.39	1.04
6:T:560:MET:CA	6:T:1767:PHE:CZ	2.39	1.04
6:T:560:MET:O	6:T:1767:PHE:HE1	1.42	1.03
6:T:480:ARG:NH1	6:T:1760:TYR:HD1	1.55	1.02
6:T:2116:LEU:HD23	6:T:2116:LEU:H	1.22	1.02
6:T:611:TYR:CE1	6:T:1583:LYS:O	2.12	1.02
6:T:694:ASP:OD1	6:T:1585:ARG:NH1	1.91	1.02
6:T:2320:LEU:HD12	6:T:2355:MET:CB	1.84	1.01
6:T:560:MET:CG	6:T:1767:PHE:CE1	2.43	1.01
6:T:2320:LEU:HD11	6:T:2356:SER:N	1.74	1.00
6:T:2276:THR:HG23	6:T:2277:PRO:CD	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:NH1	6:T:1760:TYR:CD1	2.28	0.99
6:T:480:ARG:NH1	6:T:1760:TYR:HB2	1.77	0.99
6:T:629:GLU:OE1	6:T:1717:GLN:HB3	1.60	0.99
6:T:1487:MET:HE2	6:T:1487:MET:HA	1.43	0.98
6:T:339:GLU:CD	6:T:1897:GLU:HG2	1.88	0.97
6:T:480:ARG:C	6:T:1760:TYR:OH	2.08	0.96
6:T:2320:LEU:CD1	6:T:2355:MET:CA	2.43	0.96
6:T:378:GLY:O	6:T:1856:HIS:NE2	1.99	0.96
6:T:2320:LEU:HD21	6:T:2358:SER:HG	1.27	0.95
6:T:1832:LYS:HE2	6:T:1832:LYS:HA	1.49	0.94
6:T:2320:LEU:CD1	6:T:2355:MET:HB2	1.96	0.94
6:T:694:ASP:OD2	6:T:1585:ARG:CZ	2.16	0.94
6:T:1751:SER:HB2	6:T:1796:LEU:HG	1.48	0.94
6:T:1950:THR:OG1	6:T:1951:PRO:HD3	1.69	0.92
6:T:2325:LEU:HD21	6:T:2329:ARG:HA	0.93	0.92
6:T:629:GLU:HG2	6:T:1720:GLN:OE1	1.69	0.92
6:T:2320:LEU:CD2	6:T:2358:SER:OG	2.17	0.92
6:T:560:MET:HA	6:T:1767:PHE:HZ	0.97	0.92
6:T:1547:MET:HA	6:T:1550:LYS:HE2	1.50	0.92
6:T:2325:LEU:CD2	6:T:2329:ARG:CA	2.35	0.91
6:T:694:ASP:OD2	6:T:1585:ARG:NE	2.04	0.91
6:T:2276:THR:HG23	6:T:2277:PRO:HD3	0.96	0.91
6:T:2320:LEU:HD12	6:T:2355:MET:HB2	1.47	0.91
6:T:1915:LYS:HA	6:T:1915:LYS:HE2	1.52	0.91
6:T:560:MET:HA	6:T:1767:PHE:CE1	2.05	0.91
6:T:2320:LEU:HD11	6:T:2355:MET:CA	2.01	0.91
6:T:560:MET:CG	6:T:1767:PHE:CZ	2.55	0.90
6:T:2155:GLU:HA	6:T:2158:LEU:HD13	1.54	0.89
6:T:2004:ILE:HG21	6:T:2035:ILE:HD13	1.55	0.89
6:T:1416:ILE:HD13	6:T:1459:THR:OG1	1.72	0.89
6:T:1594:THR:HG1	6:T:1595:PRO:HD3	1.31	0.88
6:T:1628:VAL:HG13	6:T:1675:THR:HG21	1.55	0.88
6:T:2155:GLU:HG3	6:T:2158:LEU:HD22	1.56	0.88
6:T:2207:GLN:HA	6:T:2210:LEU:HD12	1.54	0.88
6:T:560:MET:CA	6:T:1767:PHE:CE1	2.57	0.88
6:T:560:MET:C	6:T:1767:PHE:HE1	1.81	0.88
6:T:2115:GLU:OE1	6:T:2115:GLU:N	2.08	0.86
6:T:572:LEU:HA	6:T:1940:TYR:CD2	2.11	0.86
6:T:1553:VAL:HG12	6:T:1592:PHE:HB3	1.56	0.86
6:T:2315:LEU:HD12	6:T:2315:LEU:O	1.76	0.86
6:T:1692:ILE:HA	6:T:1695:LEU:HD12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:284:ALA:HB1	4:E:265:GLU:HG2	1.56	0.85
6:T:381:PHE:HD2	6:T:1859:LEU:HD21	1.39	0.85
6:T:381:PHE:CD2	6:T:1859:LEU:HD21	2.11	0.85
3:D:621:MET:HB3	6:T:2417:GLU:HG3	1.59	0.85
6:T:1799:ARG:N	6:T:1799:ARG:HD2	1.90	0.85
6:T:1493:GLN:HA	6:T:1493:GLN:HE21	1.41	0.85
6:T:572:LEU:CA	6:T:1940:TYR:CD2	2.60	0.84
6:T:1655:ILE:HG12	6:T:1662:VAL:HG12	1.59	0.84
6:T:1995:LEU:HD23	6:T:1995:LEU:H	1.43	0.84
6:T:2325:LEU:HD23	6:T:2329:ARG:HA	1.57	0.83
6:T:560:MET:HG2	6:T:1767:PHE:CD1	2.13	0.83
6:T:2206:LEU:HD12	6:T:2206:LEU:O	1.78	0.83
6:T:2226:ILE:HD12	6:T:2228:GLU:HB2	1.60	0.83
6:T:2239:LEU:HD11	6:T:2259:LEU:HD13	1.60	0.82
6:T:2243:ILE:HG21	6:T:2256:GLY:HA3	1.59	0.82
6:T:1296:LEU:HD13	6:T:1307:CYS:HB2	1.61	0.82
6:T:1449:LEU:HD22	6:T:1484:PRO:CG	2.09	0.82
6:T:1562:LEU:HD12	6:T:1563:PRO:HD2	1.60	0.82
6:T:1801:PHE:HA	6:T:1804:LYS:HD2	1.62	0.82
6:T:2517:LEU:HD12	6:T:2519:LEU:HB2	1.63	0.81
3:D:62:ARG:HD2	3:D:65:ILE:HB	1.61	0.81
6:T:382:THR:HG23	6:T:1900:LEU:HD11	1.63	0.81
6:T:1594:THR:OG1	6:T:1595:PRO:CD	2.28	0.81
6:T:611:TYR:OH	6:T:1583:LYS:O	1.99	0.81
6:T:560:MET:O	6:T:1767:PHE:CE1	2.33	0.80
6:T:1654:ASN:HA	6:T:1657:LYS:HE2	1.63	0.80
2:B:244:GLU:O	3:D:75:ARG:NH2	2.14	0.80
6:T:838:LEU:HD11	6:T:1251:GLU:HB3	1.64	0.80
6:T:1586:LEU:O	6:T:1586:LEU:HD23	1.83	0.79
6:T:750:ASP:HB2	6:T:753:ASN:HB2	1.64	0.79
6:T:1535:LEU:HD13	6:T:1583:LYS:HE3	1.64	0.79
6:T:1441:LEU:HB2	6:T:1473:LEU:CD1	2.13	0.79
6:T:1979:SER:HA	6:T:1983:ASN:HB2	1.64	0.79
2:B:398:VAL:HA	2:B:401:ARG:HE	1.47	0.79
4:E:246:ARG:NH1	4:E:254:GLU:OE1	2.16	0.79
6:T:799:SER:HB2	6:T:805:PRO:HB3	1.65	0.79
6:T:1487:MET:HE2	6:T:1487:MET:CA	2.12	0.78
6:T:518:MET:SD	6:T:2317:ILE:HD13	2.23	0.78
3:D:529:LEU:N	3:D:556:GLU:OE2	2.16	0.78
6:T:2168:LEU:HD12	6:T:2212:VAL:HG12	1.63	0.78
6:T:560:MET:C	6:T:1767:PHE:CE1	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1493:GLN:HA	6:T:1493:GLN:NE2	1.97	0.78
6:T:1885:ASP:HA	6:T:1888:LYS:HE3	1.65	0.78
6:T:2116:LEU:H	6:T:2116:LEU:CD2	1.97	0.77
6:T:680:ARG:HA	6:T:683:MET:HE2	1.66	0.77
6:T:2493:CYS:SG	6:T:2494:LEU:N	2.57	0.77
6:T:573:PRO:HG3	6:T:1940:TYR:CE1	2.20	0.77
6:T:1832:LYS:HE2	6:T:1832:LYS:CA	2.15	0.77
6:T:1562:LEU:CD1	6:T:1563:PRO:HD2	2.13	0.77
6:T:2271:ILE:HG21	6:T:2274:LEU:HD12	1.66	0.77
1:A:188:TYR:HB2	1:A:267:LEU:HD21	1.66	0.77
6:T:773:VAL:HG21	6:T:784:LEU:HD12	1.67	0.77
6:T:2688:THR:OG1	6:T:2729:TRP:NE1	2.17	0.77
6:T:730:GLU:HG2	6:T:732:THR:H	1.50	0.76
6:T:340:LEU:O	6:T:344:ARG:NH1	2.18	0.76
6:T:2007:ILE:HG13	6:T:2031:LEU:HD22	1.66	0.76
6:T:3688:LEU:HA	6:T:3691:MET:HE2	1.67	0.76
6:T:351:THR:HA	6:T:354:ILE:HD12	1.67	0.76
6:T:572:LEU:C	6:T:1940:TYR:CE2	2.64	0.76
6:T:1635:GLU:H	6:T:1635:GLU:CD	1.93	0.75
6:T:480:ARG:CG	6:T:1760:TYR:CE1	2.69	0.75
6:T:956:ASN:HD21	6:T:2843:LEU:HB3	1.52	0.75
6:T:2241:SER:HA	6:T:2274:LEU:HD21	1.68	0.75
6:T:3412:HIS:NE2	6:T:3585:GLU:OE1	2.20	0.75
6:T:1543:LEU:H	6:T:1543:LEU:CD2	1.96	0.74
6:T:1789:PHE:HB3	6:T:1803:LEU:HD13	1.69	0.74
6:T:570:LEU:HG	6:T:1940:TYR:HE2	1.50	0.74
6:T:1971:LYS:HE2	6:T:2000:ARG:HG3	1.68	0.74
3:D:62:ARG:NH1	3:D:65:ILE:O	2.21	0.74
6:T:2278:LEU:C	6:T:2278:LEU:HD12	2.12	0.74
6:T:1766:ILE:HD13	6:T:1769:ASN:HD21	1.52	0.74
6:T:1506:LEU:C	6:T:1506:LEU:HD12	2.13	0.74
6:T:2986:ARG:HH12	6:T:3055:LYS:HE2	1.53	0.74
6:T:3043:PHE:HB3	6:T:3060:TRP:HE3	1.52	0.74
6:T:1449:LEU:CD2	6:T:1484:PRO:HG2	2.15	0.73
6:T:1463:LEU:O	6:T:1463:LEU:HD23	1.89	0.73
6:T:1473:LEU:HD23	6:T:1473:LEU:C	2.14	0.73
5:F:633:GLU:OE2	5:F:655:ASN:ND2	2.21	0.73
6:T:2090:LEU:HD12	6:T:2093:ARG:HB2	1.70	0.73
6:T:2245:GLN:HA	6:T:2245:GLN:NE2	2.04	0.73
6:T:1543:LEU:HD22	6:T:1543:LEU:N	2.01	0.73
6:T:1762:LEU:HD23	6:T:1762:LEU:C	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2100:LEU:HD23	6:T:2100:LEU:C	2.14	0.73
6:T:2116:LEU:HD23	6:T:2116:LEU:N	2.02	0.73
6:T:2329:ARG:HH22	6:T:2367:PRO:HD2	1.53	0.73
3:D:45:CYS:SG	6:T:3497:HIS:NE2	2.62	0.73
6:T:560:MET:CA	6:T:1767:PHE:HZ	1.86	0.73
6:T:1006:SER:O	6:T:1014:ARG:NH1	2.22	0.73
6:T:1854:LEU:HD23	6:T:1854:LEU:C	2.14	0.73
6:T:2034:LEU:HD23	6:T:2034:LEU:C	2.14	0.72
6:T:2124:LEU:HD23	6:T:2124:LEU:C	2.14	0.72
6:T:3054:ALA:H	6:T:3091:LEU:HD22	1.53	0.72
6:T:1907:LEU:HD23	6:T:1907:LEU:C	2.14	0.72
2:B:467:GLN:HA	4:E:85:ALA:HB1	1.71	0.72
6:T:917:ILE:HG12	6:T:921:ILE:HG12	1.70	0.72
6:T:65:SER:HA	6:T:76:ARG:HH22	1.54	0.72
6:T:2282:PHE:HB2	6:T:2315:LEU:HD21	1.70	0.72
6:T:2957:HIS:HA	6:T:3434:VAL:HG11	1.72	0.72
1:A:332:PRO:O	1:A:335:ARG:NE	2.23	0.72
6:T:339:GLU:OE2	6:T:1897:GLU:HG2	1.90	0.72
6:T:1482:LEU:HD12	6:T:1485:LEU:HB2	1.70	0.72
6:T:2354:ASN:OD1	6:T:2357:ARG:NH1	2.21	0.72
1:A:107:GLU:OE1	1:A:116:ARG:NH1	2.23	0.71
1:A:285:CYS:SG	1:A:286:ASP:N	2.63	0.71
6:T:381:PHE:CB	6:T:1858:ASP:OD1	2.36	0.71
6:T:1535:LEU:HD23	6:T:1535:LEU:C	2.14	0.71
6:T:2976:ILE:HB	6:T:2980:GLU:HB2	1.71	0.71
6:T:1703:LEU:HD23	6:T:1703:LEU:C	2.15	0.71
6:T:3054:ALA:HB2	6:T:3091:LEU:HB3	1.70	0.71
6:T:2649:ILE:HD12	6:T:2655:ILE:HD13	1.72	0.71
6:T:339:GLU:OE1	6:T:1897:GLU:HG2	1.88	0.71
6:T:1586:LEU:HD23	6:T:1586:LEU:C	2.15	0.71
6:T:1850:ALA:HB1	6:T:1860:PHE:HE2	1.54	0.71
6:T:2138:VAL:HA	6:T:2142:TYR:HB2	1.73	0.71
6:T:560:MET:CB	6:T:1767:PHE:CZ	2.74	0.71
6:T:1919:PRO:HG2	6:T:1922:VAL:HB	1.71	0.71
6:T:1949:LEU:HD23	6:T:1949:LEU:C	2.15	0.71
6:T:2811:GLN:HG3	6:T:2814:ARG:HD3	1.73	0.71
6:T:1699:LEU:O	6:T:1699:LEU:HD23	1.90	0.71
6:T:1995:LEU:H	6:T:1995:LEU:CD2	2.02	0.71
6:T:1600:LEU:HD13	6:T:1607:VAL:HG11	1.73	0.70
6:T:339:GLU:CD	6:T:1897:GLU:CG	2.64	0.70
6:T:1593:ARG:HG2	6:T:1627:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1829:LYS:O	6:T:1829:LYS:HD3	1.91	0.70
3:D:768:MET:HA	3:D:771:ARG:HG2	1.73	0.70
6:T:2613:ILE:HG21	6:T:2616:LEU:HB2	1.72	0.70
2:B:394:MET:SD	2:B:401:ARG:NH1	2.65	0.70
6:T:1570:LEU:HD23	6:T:1570:LEU:C	2.17	0.70
6:T:1619:GLN:OE1	6:T:1619:GLN:N	2.18	0.70
6:T:1872:ILE:HD11	6:T:1886:ILE:HG21	1.73	0.70
3:D:623:TYR:HB2	3:D:626:ARG:HE	1.54	0.70
6:T:570:LEU:HD11	6:T:1940:TYR:OH	1.92	0.70
6:T:629:GLU:OE2	6:T:1717:GLN:HB3	1.91	0.70
6:T:2118:LEU:C	6:T:2118:LEU:HD23	2.16	0.70
3:D:35:GLU:OE1	6:T:3731:ARG:NH2	2.25	0.70
6:T:480:ARG:NH1	6:T:1760:TYR:CB	2.55	0.70
6:T:1794:LYS:H	6:T:1794:LYS:HD3	1.56	0.70
6:T:1941:LEU:HD12	6:T:1941:LEU:O	1.92	0.70
4:E:86:ASN:HB2	4:E:89:VAL:HG22	1.74	0.69
6:T:572:LEU:N	6:T:1940:TYR:CD2	2.60	0.69
6:T:3715:VAL:HG23	6:T:3716:THR:H	1.56	0.69
6:T:1718:LEU:C	6:T:1718:LEU:HD12	2.18	0.69
6:T:1716:LEU:H	6:T:1716:LEU:CD1	1.94	0.69
6:T:1995:LEU:HD23	6:T:1995:LEU:N	2.07	0.69
6:T:2031:LEU:HD12	6:T:2031:LEU:O	1.93	0.69
3:D:614:GLN:HB2	6:T:2456:ARG:HH12	1.56	0.69
6:T:222:LYS:NZ	6:T:238:TYR:OH	2.24	0.69
6:T:1879:ILE:HB	6:T:1882:ILE:HG12	1.75	0.69
6:T:1915:LYS:HE2	6:T:1915:LYS:CA	2.22	0.69
6:T:2093:ARG:HG2	6:T:2127:LEU:HD11	1.72	0.69
6:T:2325:LEU:HD21	6:T:2329:ARG:N	2.07	0.69
6:T:2320:LEU:O	6:T:2320:LEU:HD23	1.92	0.69
1:A:16:MET:O	1:A:18:LYS:NZ	2.26	0.69
3:D:33:ILE:HD12	3:D:300:ILE:HD11	1.74	0.69
3:D:45:CYS:HG	6:T:3497:HIS:CE1	2.11	0.69
3:D:617:LYS:O	3:D:619:ARG:NH1	2.26	0.69
6:T:966:LEU:HD12	6:T:3540:ASP:HB2	1.72	0.69
6:T:2303:GLU:OE1	6:T:2303:GLU:N	2.19	0.69
6:T:474:ARG:O	6:T:474:ARG:NH2	2.26	0.69
6:T:2320:LEU:HD11	6:T:2355:MET:O	1.90	0.69
2:B:441:THR:OG1	2:B:448:ARG:NH2	2.27	0.68
6:T:1100:MET:O	6:T:1104:ASN:ND2	2.25	0.68
6:T:2168:LEU:HD23	6:T:2168:LEU:C	2.19	0.68
6:T:1900:LEU:H	6:T:1900:LEU:CD2	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:339:GLU:OE1	6:T:1897:GLU:CG	2.41	0.68
6:T:481:GLN:N	6:T:1760:TYR:OH	2.27	0.68
6:T:1204:GLU:OE1	6:T:3373:ARG:NH1	2.26	0.68
6:T:1300:ASN:HB3	6:T:1303:VAL:HG12	1.76	0.68
6:T:2128:ILE:HG21	6:T:2173:LYS:HB3	1.75	0.68
6:T:3446:PRO:HD3	6:T:3582:PHE:HB2	1.75	0.68
3:D:312:THR:OG1	6:T:3629:GLN:NE2	2.27	0.68
6:T:613:VAL:CG1	6:T:1536:ASP:OD1	2.38	0.68
6:T:1472:LYS:HG3	6:T:1475:LYS:HE2	1.74	0.68
1:A:93:GLU:HG3	1:A:94:LEU:HD12	1.75	0.68
3:D:657:GLU:O	3:D:661:ASN:ND2	2.23	0.68
6:T:613:VAL:HA	6:T:1536:ASP:OD2	1.94	0.68
6:T:1577:VAL:HG13	6:T:1592:PHE:HE2	1.59	0.68
6:T:2342:HIS:HB3	6:T:2344:MET:HE3	1.75	0.68
3:D:670:GLU:OE1	3:D:670:GLU:N	2.26	0.68
6:T:1920:ILE:HD12	6:T:1920:ILE:N	2.04	0.68
6:T:727:LEU:HG	6:T:772:SER:HB3	1.76	0.68
6:T:2955:ARG:HH12	6:T:2990:LYS:HB3	1.59	0.68
1:A:196:ARG:HH12	1:A:250:ILE:HA	1.57	0.67
6:T:2039:GLU:HA	6:T:2039:GLU:OE1	1.94	0.67
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.76	0.67
4:E:289:GLN:NE2	4:E:291:ILE:O	2.27	0.67
6:T:1361:LEU:HD23	6:T:1421:ILE:HG23	1.76	0.67
6:T:1509:LEU:HD22	6:T:1509:LEU:N	2.09	0.67
2:B:47:TYR:OH	2:B:66:ARG:NH2	2.28	0.67
6:T:515:GLU:HA	6:T:518:MET:HE2	1.75	0.67
6:T:2244:THR:HG21	6:T:2274:LEU:HD22	1.77	0.67
6:T:1476:GLU:N	6:T:1476:GLU:OE1	2.28	0.67
6:T:1482:LEU:HG	6:T:1486:LEU:HG	1.77	0.67
2:B:243:LYS:NZ	7:B:501:ATP:O2'	2.28	0.67
1:A:35:VAL:HA	1:A:54:VAL:HG12	1.77	0.67
3:D:48:ARG:HG2	3:D:55:LEU:HD13	1.77	0.67
5:F:537:ASN:O	5:F:538:LEU:HG	1.95	0.67
6:T:2303:GLU:H	6:T:2303:GLU:CD	2.02	0.67
2:B:112:GLU:OE1	2:B:116:ASN:ND2	2.25	0.67
6:T:1378:LEU:HD12	6:T:1415:CYS:HB2	1.77	0.67
6:T:2387:GLU:OE1	6:T:2390:LEU:N	2.22	0.67
4:E:293:GLN:OE1	4:E:302:GLN:NE2	2.28	0.67
6:T:110:GLU:HG2	6:T:214:LEU:HD13	1.76	0.67
6:T:1941:LEU:HA	6:T:1944:GLN:HE21	1.60	0.66
6:T:2008:ILE:HG12	6:T:2031:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2320:LEU:HD13	6:T:2355:MET:CA	2.19	0.66
6:T:469:ASP:O	6:T:473:ASN:ND2	2.28	0.66
6:T:2179:TRP:HA	6:T:2181:MET:HE1	1.78	0.66
6:T:1777:GLU:OE1	6:T:1777:GLU:HA	1.94	0.66
6:T:1936:VAL:HA	6:T:1939:ARG:HG3	1.77	0.66
6:T:141:ILE:HA	6:T:144:ILE:HD12	1.76	0.66
6:T:968:GLU:OE1	6:T:968:GLU:N	2.29	0.66
6:T:1577:VAL:HG21	6:T:1596:LEU:HD11	1.76	0.66
6:T:1936:VAL:HG23	6:T:1939:ARG:HD3	1.77	0.66
6:T:1485:LEU:HD22	6:T:1503:LEU:HD21	1.77	0.66
6:T:2485:GLU:HG2	6:T:2486:LEU:H	1.61	0.66
5:F:637:LYS:NZ	5:F:654:PRO:O	2.28	0.66
6:T:2014:ILE:HG13	6:T:2024:SER:HB2	1.77	0.66
6:T:1737:GLU:H	6:T:1737:GLU:CD	2.04	0.66
6:T:1881:GLU:H	6:T:1881:GLU:CD	2.04	0.66
6:T:2773:ARG:HA	6:T:2776:LEU:HB2	1.78	0.66
6:T:1178:ILE:HD12	6:T:2519:LEU:HD23	1.78	0.65
6:T:1179:TYR:HD2	6:T:1184:ALA:HA	1.61	0.65
6:T:1900:LEU:HD23	6:T:1900:LEU:N	2.01	0.65
6:T:943:HIS:NE2	6:T:2818:ASP:OD1	2.24	0.65
6:T:2184:LEU:HD23	6:T:2184:LEU:C	2.21	0.65
6:T:1315:SER:O	6:T:1319:GLY:HA2	1.94	0.65
6:T:2325:LEU:HD11	6:T:2328:SER:HB3	1.78	0.65
3:D:274:ASN:OD1	3:D:275:ASP:N	2.29	0.65
1:A:153:LEU:HD23	1:A:299:MET:HE1	1.78	0.65
6:T:1538:LEU:HD22	6:T:1546:GLN:HE22	1.61	0.65
6:T:1546:GLN:HG3	6:T:1548:PRO:HD2	1.79	0.65
6:T:1815:VAL:HG21	6:T:1870:ILE:HD11	1.79	0.65
6:T:2450:ARG:NH1	6:T:2475:LEU:O	2.30	0.65
6:T:2315:LEU:HD12	6:T:2315:LEU:C	2.22	0.65
6:T:2604:ASN:HD22	6:T:2632:ALA:HB2	1.62	0.65
6:T:1689:GLY:HA2	6:T:1692:ILE:HG23	1.77	0.65
3:D:45:CYS:O	6:T:3497:HIS:NE2	2.30	0.65
6:T:572:LEU:N	6:T:1940:TYR:HD2	1.95	0.65
6:T:1036:PRO:HD3	6:T:2498:SER:HA	1.79	0.65
6:T:1662:VAL:HG11	6:T:1705:THR:HG21	1.78	0.65
6:T:1840:LYS:HD2	6:T:1840:LYS:C	2.22	0.65
6:T:382:THR:HG22	6:T:1858:ASP:OD2	1.96	0.65
6:T:2184:LEU:HD23	6:T:2184:LEU:O	1.97	0.65
2:B:71:LEU:HD11	2:B:229:LEU:HD23	1.79	0.65
6:T:944:ASN:OD1	6:T:947:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:533:GLU:OE1	3:D:533:GLU:N	2.29	0.64
6:T:813:ARG:HD3	6:T:817:ARG:HD3	1.79	0.64
6:T:1797:ASP:HA	6:T:1800:ILE:HD12	1.79	0.64
6:T:2464:ALA:HA	6:T:2596:ILE:HA	1.78	0.64
2:B:20:ASP:OD2	2:B:452:SER:OG	2.14	0.64
6:T:780:ASN:HB2	6:T:782:VAL:HG12	1.77	0.64
6:T:1848:ILE:HG21	6:T:1852:ASP:H	1.63	0.64
6:T:2803:PHE:HA	6:T:2809:GLY:HA3	1.78	0.64
6:T:2177:LYS:HZ3	6:T:2179:TRP:HB3	1.62	0.64
6:T:2369:VAL:O	6:T:2415:ARG:NH1	2.29	0.64
6:T:466:ILE:HA	6:T:1716:LEU:HD21	1.80	0.64
6:T:1939:ARG:HB3	6:T:1939:ARG:CZ	2.26	0.64
6:T:2271:ILE:HG12	6:T:2274:LEU:HG	1.80	0.64
6:T:2421:LEU:HD13	6:T:2460:TRP:HB2	1.78	0.64
3:D:615:LEU:HD21	6:T:2452:TYR:HB3	1.79	0.64
5:F:588:ILE:HD11	5:F:593:ARG:HH21	1.63	0.64
6:T:2560:TRP:CD1	6:T:2609:SER:HG	2.16	0.64
6:T:2768:ASP:OD1	6:T:2769:TRP:N	2.31	0.64
1:A:66:THR:OG1	1:A:68:ARG:NH2	2.27	0.64
1:A:154:ASP:HA	1:A:300:SER:O	1.96	0.64
1:A:334:GLU:OE1	1:A:334:GLU:N	2.30	0.64
5:F:581:LEU:HD23	5:F:615:LYS:HE3	1.79	0.64
6:T:1265:ILE:HG23	6:T:1313:THR:HG21	1.79	0.64
6:T:1567:ASP:HB3	6:T:1569:PHE:HD2	1.61	0.64
6:T:1634:LYS:HD2	6:T:1634:LYS:C	2.22	0.64
6:T:2792:GLN:HG2	6:T:2820:GLY:HA2	1.78	0.64
6:T:1881:GLU:OE1	6:T:1881:GLU:N	2.19	0.64
6:T:1821:LEU:HB3	6:T:1874:ALA:HB1	1.78	0.64
6:T:2869:ASN:O	6:T:2872:SER:OG	2.15	0.64
2:B:93:ALA:O	2:B:97:GLU:HB2	1.97	0.64
6:T:1757:LYS:HZ1	6:T:1802:VAL:HG13	1.63	0.64
6:T:2680:ARG:HE	6:T:2689:ASN:HD22	1.44	0.64
6:T:3004:ASP:O	6:T:3008:ASN:N	2.30	0.64
3:D:561:GLN:OE1	3:D:561:GLN:N	2.31	0.63
4:E:269:LYS:O	4:E:270:ARG:NE	2.31	0.63
6:T:1877:GLU:CD	6:T:1877:GLU:H	2.05	0.63
6:T:2276:THR:CG2	6:T:2277:PRO:CD	2.63	0.63
6:T:2632:ALA:HB1	6:T:2635:GLN:HB2	1.79	0.63
6:T:934:PRO:HB3	6:T:2825:LEU:HB3	1.81	0.63
3:D:303:ILE:HD13	3:D:315:ILE:HD13	1.79	0.63
6:T:570:LEU:HG	6:T:1940:TYR:CE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:626:PHE:O	6:T:1587:GLN:NE2	2.31	0.63
6:T:1854:LEU:HD23	6:T:1854:LEU:O	1.97	0.63
3:D:347:ARG:NH1	3:D:582:PHE:O	2.32	0.63
6:T:2373:ALA:HA	6:T:2376:LEU:HD12	1.80	0.63
2:B:152:ARG:NH1	2:B:407:ASN:OD1	2.32	0.63
6:T:336:CYS:HB2	6:T:344:ARG:HH21	1.62	0.63
1:A:14:SER:HB2	1:A:158:GLY:H	1.63	0.63
4:E:84:LYS:HG2	4:E:90:THR:HG22	1.79	0.63
6:T:1529:TRP:HB3	6:T:1552:ILE:HD11	1.80	0.63
6:T:1203:ASP:OD1	6:T:1204:GLU:N	2.32	0.63
6:T:1476:GLU:HG2	6:T:1477:LEU:HD22	1.81	0.63
6:T:2590:PRO:HG2	6:T:2592:HIS:CE1	2.33	0.63
6:T:3060:TRP:O	6:T:3064:ASN:ND2	2.32	0.63
6:T:148:TYR:OH	6:T:218:MET:SD	2.54	0.63
6:T:956:ASN:ND2	6:T:2843:LEU:O	2.31	0.63
6:T:1879:ILE:HG13	6:T:1879:ILE:O	1.99	0.63
6:T:2680:ARG:NH1	6:T:3638:GLU:OE2	2.31	0.63
6:T:480:ARG:CA	6:T:1760:TYR:OH	2.46	0.62
6:T:615:ASN:HB3	6:T:618:LEU:HD13	1.80	0.62
6:T:856:GLU:HA	6:T:859:VAL:HG12	1.80	0.62
6:T:1304:ARG:HH11	6:T:1352:GLY:HA2	1.63	0.62
6:T:1487:MET:HA	6:T:1487:MET:CE	2.26	0.62
6:T:3357:GLN:HE22	6:T:3369:ILE:H	1.47	0.62
6:T:3505:ASP:OD2	6:T:3508:ILE:N	2.30	0.62
1:A:97:ALA:O	1:A:101:HIS:NE2	2.32	0.62
6:T:612:THR:OG1	6:T:1583:LYS:NZ	2.32	0.62
6:T:2704:GLN:HG3	6:T:2733:TRP:HE1	1.62	0.62
6:T:2773:ARG:NH1	6:T:2802:ASN:OD1	2.33	0.62
1:A:205:GLU:HA	1:A:208:ILE:HG22	1.81	0.62
2:B:44:TYR:HB3	2:B:74:ILE:HD11	1.82	0.62
3:D:33:ILE:O	3:D:36:ARG:HD3	2.00	0.62
4:E:98:SER:OG	4:E:100:GLU:OE1	2.18	0.62
6:T:568:PRO:HG2	6:T:569:ILE:HD12	1.80	0.62
6:T:767:LYS:O	6:T:771:MET:HG2	1.99	0.62
6:T:3244:ASP:OD1	6:T:3247:ARG:NH2	2.32	0.62
6:T:3410:VAL:HB	6:T:3412:HIS:CE1	2.34	0.62
1:A:196:ARG:HD3	1:A:198:TYR:HE2	1.64	0.62
6:T:2329:ARG:HH11	6:T:2368:THR:HG22	1.63	0.62
6:T:3122:ASP:OD1	6:T:3123:SER:N	2.31	0.62
6:T:3589:SER:OG	6:T:3615:HIS:O	2.17	0.62
2:B:119:GLU:HA	2:B:122:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:339:GLU:HA	6:T:1898:ASP:OD1	1.99	0.62
6:T:2320:LEU:HD23	6:T:2320:LEU:C	2.25	0.62
1:A:141:SER:HB3	1:A:339:VAL:HG12	1.82	0.62
3:D:550:ASP:OD2	5:F:652:ARG:NH1	2.32	0.62
6:T:1053:GLU:HG2	6:T:1054:ARG:HG2	1.81	0.62
6:T:3096:LYS:HD2	6:T:3428:LYS:HG2	1.81	0.62
6:T:3737:ASP:OD1	6:T:3738:VAL:N	2.33	0.62
6:T:1771:ILE:HD12	6:T:1814:GLU:HB2	1.82	0.62
6:T:1884:LYS:HA	6:T:1887:ILE:HD12	1.82	0.62
6:T:2690:ILE:HA	6:T:3715:VAL:HA	1.82	0.62
6:T:114:ASN:O	6:T:215:ARG:NH1	2.33	0.62
6:T:2302:GLU:OE2	6:T:2302:GLU:N	2.20	0.62
6:T:2004:ILE:HD13	6:T:2035:ILE:HD13	1.82	0.62
6:T:3578:SER:OG	6:T:3580:ASN:ND2	2.33	0.62
6:T:21:LEU:HD12	6:T:24:ARG:HH12	1.65	0.61
6:T:2762:CYS:SG	6:T:2763:GLY:N	2.72	0.61
6:T:560:MET:HG2	6:T:1767:PHE:CE2	2.31	0.61
6:T:2537:ILE:HG22	6:T:2539:SER:H	1.65	0.61
6:T:2688:THR:HG1	6:T:2729:TRP:HE1	1.46	0.61
6:T:3306:ASP:OD1	6:T:3309:THR:N	2.32	0.61
1:A:304:THR:O	1:A:335:ARG:NH1	2.32	0.61
6:T:1030:LYS:NZ	6:T:2485:GLU:O	2.33	0.61
6:T:1776:LYS:HG2	6:T:1776:LYS:O	1.99	0.61
3:D:70:LYS:HD3	3:D:540:ALA:HB2	1.82	0.61
3:D:378:LYS:NZ	3:D:536:LYS:O	2.30	0.61
6:T:1562:LEU:CG	6:T:1563:PRO:HD2	2.29	0.61
6:T:1585:ARG:O	6:T:1585:ARG:HG3	2.00	0.61
6:T:3540:ASP:OD1	6:T:3541:PHE:N	2.33	0.61
6:T:355:LEU:HD13	6:T:364:LEU:HD13	1.83	0.61
6:T:413:LYS:HG3	6:T:416:LYS:HE3	1.81	0.61
6:T:1737:GLU:OE1	6:T:1737:GLU:N	2.19	0.61
5:F:551:LEU:HD13	5:F:627:LEU:HD22	1.81	0.61
6:T:249:PHE:O	6:T:288:ARG:NH1	2.34	0.61
6:T:1903:GLN:HE21	6:T:1941:LEU:HG	1.66	0.61
6:T:2184:LEU:N	6:T:2185:PRO:HD2	2.14	0.61
6:T:2552:ASP:OD2	6:T:2555:ALA:N	2.30	0.61
6:T:1438:ILE:HA	6:T:1473:LEU:CD1	2.31	0.61
6:T:1543:LEU:HG	6:T:1591:PRO:HG3	1.83	0.61
6:T:3400:VAL:O	6:T:3401:HIS:ND1	2.34	0.61
3:D:293:MET:HE1	4:E:272:LEU:HD13	1.83	0.61
4:E:243:LEU:HD23	4:E:246:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1340:LYS:NZ	6:T:1344:ALA:O	2.33	0.61
6:T:1800:ILE:HG22	6:T:1804:LYS:HE3	1.83	0.61
6:T:2546:ILE:HA	6:T:2549:PHE:HD2	1.64	0.61
2:B:481:GLU:O	2:B:485:ASN:ND2	2.33	0.61
6:T:1619:GLN:H	6:T:1619:GLN:CD	2.07	0.61
3:D:649:ILE:HG13	3:D:688:ILE:HD12	1.82	0.60
6:T:1449:LEU:HD13	6:T:1484:PRO:HB2	1.83	0.60
6:T:1574:LEU:HD22	6:T:1623:PHE:HE2	1.65	0.60
6:T:2007:ILE:HD11	6:T:2031:LEU:HD13	1.83	0.60
6:T:3008:ASN:O	6:T:3010:ASN:ND2	2.34	0.60
6:T:10:PHE:HB2	6:T:13:ARG:NE	2.16	0.60
6:T:1337:ILE:HG23	6:T:1353:ASN:HB3	1.83	0.60
2:B:463:GLY:HA2	2:B:466:HIS:HE1	1.67	0.60
6:T:2324:LEU:O	6:T:2324:LEU:HD12	2.01	0.60
6:T:306:ALA:HA	6:T:309:PHE:CE2	2.35	0.60
6:T:422:LEU:HD13	6:T:432:GLN:HB3	1.83	0.60
6:T:466:ILE:HG12	6:T:1716:LEU:HD11	1.83	0.60
6:T:1463:LEU:HD23	6:T:1463:LEU:C	2.26	0.60
6:T:2175:LYS:HD3	6:T:2175:LYS:N	2.16	0.60
6:T:2465:ASP:OD1	6:T:2466:TYR:N	2.34	0.60
1:A:200:PHE:HD1	1:A:205:GLU:HB2	1.65	0.60
3:D:323:ARG:HH12	5:F:561:PRO:HD3	1.67	0.60
3:D:649:ILE:H	3:D:688:ILE:HG23	1.67	0.60
3:D:719:SER:O	3:D:722:GLN:NE2	2.33	0.60
6:T:693:MET:HG3	6:T:694:ASP:H	1.66	0.60
6:T:957:ARG:NH2	6:T:2893:ASP:OD2	2.33	0.60
6:T:1179:TYR:HB3	6:T:1183:LEU:HG	1.84	0.60
6:T:1300:ASN:HD22	6:T:1303:VAL:H	1.50	0.60
6:T:1913:ILE:HD12	6:T:1923:VAL:HG22	1.83	0.60
6:T:2289:HIS:HA	6:T:2292:ILE:HG12	1.83	0.60
6:T:2474:GLN:OE1	6:T:2546:ILE:HD12	2.02	0.60
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.35	0.60
6:T:1897:GLU:OE1	6:T:1897:GLU:N	2.33	0.60
4:E:292:THR:HG22	4:E:295:LEU:HD12	1.84	0.60
6:T:1420:ALA:HB2	6:T:1462:ALA:HB1	1.83	0.60
6:T:1814:GLU:HG2	6:T:1821:LEU:HD12	1.84	0.60
6:T:1936:VAL:HG23	6:T:1939:ARG:HH11	1.66	0.60
6:T:1936:VAL:HG22	6:T:1936:VAL:O	2.02	0.60
6:T:2460:TRP:HD1	6:T:2462:PHE:HD1	1.49	0.60
6:T:3067:ARG:NH2	6:T:3077:PHE:O	2.35	0.60
6:T:3151:MET:SD	6:T:3151:MET:N	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:565:LEU:HB3	5:F:585:LEU:HD13	1.84	0.60
6:T:3260:TYR:HA	6:T:3307:TYR:OH	2.02	0.60
6:T:706:LEU:HG	6:T:707:PRO:HD3	1.83	0.60
6:T:1199:HIS:ND1	6:T:3333:ASN:OD1	2.35	0.60
6:T:1716:LEU:HD12	6:T:1716:LEU:N	2.01	0.60
6:T:1962:THR:OG1	6:T:1963:PRO:HD3	2.01	0.60
6:T:21:LEU:O	6:T:24:ARG:NH1	2.35	0.60
6:T:679:ALA:O	6:T:683:MET:HG3	2.00	0.60
6:T:1112:LEU:O	6:T:1115:VAL:HG12	2.01	0.60
6:T:1244:VAL:O	6:T:1248:THR:HG23	2.02	0.60
6:T:2516:ASP:OD1	6:T:2517:LEU:N	2.34	0.60
6:T:3333:ASN:HB2	6:T:3336:VAL:HG22	1.82	0.60
1:A:163:VAL:HG22	1:A:175:ILE:HG23	1.84	0.59
6:T:1672:LEU:HG	6:T:1676:MET:HE3	1.84	0.59
3:D:358:HIS:HB2	4:E:115:ASN:HA	1.84	0.59
6:T:344:ARG:HA	6:T:347:LEU:HB3	1.84	0.59
6:T:411:ILE:O	6:T:415:ILE:HG12	2.01	0.59
6:T:573:PRO:HD3	6:T:1940:TYR:CG	2.38	0.59
6:T:1957:MET:HE2	6:T:1965:THR:HB	1.84	0.59
6:T:2894:ASP:OD1	6:T:2895:VAL:N	2.36	0.59
1:A:220:ALA:O	1:A:312:ARG:NH1	2.35	0.59
2:B:467:GLN:NE2	2:B:468:LEU:HB2	2.18	0.59
6:T:110:GLU:O	6:T:215:ARG:NH1	2.31	0.59
6:T:2587:LEU:O	6:T:2594:ARG:NH2	2.36	0.59
6:T:355:LEU:HD12	6:T:398:PHE:CE1	2.37	0.59
6:T:793:LEU:HD21	6:T:831:ILE:HD11	1.83	0.59
6:T:877:PRO:HA	6:T:916:ILE:HD11	1.83	0.59
6:T:922:ASP:N	6:T:922:ASP:OD1	2.35	0.59
6:T:1825:LEU:HG	6:T:1878:ILE:HG21	1.83	0.59
6:T:1838:HIS:HE1	6:T:1882:ILE:HG23	1.67	0.59
6:T:2301:LEU:HG	6:T:2304:ALA:HB3	1.83	0.59
6:T:3155:ILE:O	6:T:3159:ILE:HG13	2.02	0.59
1:A:100:GLU:OE1	1:A:100:GLU:N	2.35	0.59
6:T:1182:GLU:OE2	6:T:1182:GLU:N	2.26	0.59
6:T:2549:PHE:HD1	6:T:2556:ILE:HG22	1.67	0.59
6:T:3397:ASP:OD1	6:T:3398:GLY:N	2.35	0.59
4:E:169:ILE:O	4:E:173:PHE:HB2	2.03	0.59
6:T:381:PHE:CB	6:T:1859:LEU:HD21	2.33	0.59
6:T:2285:LEU:HD21	6:T:2311:LEU:HD11	1.85	0.59
6:T:2477:TYR:HD2	6:T:2542:ILE:HB	1.67	0.59
1:A:282:ILE:HG23	1:A:293:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:HD2	6:T:1760:TYR:CE1	2.29	0.59
6:T:917:ILE:HG23	6:T:921:ILE:HD11	1.83	0.59
6:T:1441:LEU:CB	6:T:1473:LEU:CD1	2.81	0.59
6:T:2461:GLU:HA	6:T:2592:HIS:CG	2.37	0.59
2:B:78:GLY:O	2:B:113:PRO:HG3	2.02	0.59
6:T:619:TRP:CG	6:T:623:SER:HG	2.21	0.59
6:T:2128:ILE:HD12	6:T:2173:LYS:HG3	1.85	0.59
6:T:3472:ASN:HD22	6:T:3482:PRO:HG2	1.68	0.59
1:A:213:LYS:NZ	1:A:214:GLU:OE2	2.35	0.59
6:T:626:PHE:HB3	6:T:630:GLU:HB2	1.84	0.59
6:T:2347:ASN:OD1	6:T:2348:PHE:N	2.34	0.59
6:T:2647:THR:HG22	6:T:2648:SER:H	1.68	0.59
6:T:1438:ILE:HG23	6:T:1473:LEU:HG	1.84	0.58
6:T:1949:LEU:HG	6:T:1953:LEU:HD23	1.84	0.58
6:T:3277:GLU:O	6:T:3281:VAL:HG23	2.02	0.58
1:A:89:THR:HA	1:A:93:GLU:HB3	1.84	0.58
6:T:2090:LEU:HD12	6:T:2090:LEU:O	2.03	0.58
6:T:2229:GLU:HG3	6:T:2233:LYS:HG3	1.84	0.58
6:T:2611:SER:HA	6:T:2639:ILE:HD11	1.84	0.58
6:T:2894:ASP:OD1	6:T:2896:ASN:N	2.35	0.58
2:B:190:ILE:HD11	2:B:292:LEU:HD22	1.86	0.58
3:D:346:LYS:H	3:D:346:LYS:HD2	1.66	0.58
6:T:18:ASP:O	6:T:23:SER:OG	2.19	0.58
6:T:1350:GLN:O	6:T:1354:VAL:HG23	2.04	0.58
6:T:1793:ASP:HA	6:T:1800:ILE:HD13	1.84	0.58
2:B:416:SER:HA	2:B:448:ARG:HH11	1.68	0.58
6:T:629:GLU:CD	6:T:1717:GLN:CB	2.61	0.58
6:T:716:ASP:OD1	6:T:717:SER:N	2.36	0.58
6:T:776:PHE:HB3	6:T:779:ILE:HG22	1.85	0.58
6:T:2341:ASP:O	6:T:2385:ARG:NH1	2.36	0.58
2:B:178:LYS:N	4:E:188:ASP:OD2	2.34	0.58
6:T:837:VAL:HA	6:T:840:GLN:HE21	1.68	0.58
6:T:2851:GLU:OE1	6:T:2884:TRP:NE1	2.35	0.58
6:T:3465:THR:OG1	6:T:3466:THR:N	2.37	0.58
3:D:377:HIS:O	3:D:381:VAL:HG23	2.04	0.58
6:T:365:PRO:HG3	6:T:398:PHE:HZ	1.67	0.58
6:T:2325:LEU:HG	6:T:2329:ARG:HB3	1.85	0.58
6:T:2335:THR:O	6:T:2339:LEU:HG	2.03	0.58
6:T:2646:ASN:ND2	6:T:2647:THR:OG1	2.36	0.58
3:D:760:MET:O	3:D:764:ILE:HG12	2.04	0.58
6:T:854:GLU:OE1	6:T:854:GLU:N	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2158:LEU:H	6:T:2158:LEU:HD12	1.67	0.58
6:T:2704:GLN:O	6:T:2708:GLU:HG2	2.02	0.58
6:T:480:ARG:HB2	6:T:1760:TYR:HH	1.63	0.58
6:T:1323:VAL:HG12	6:T:1366:THR:HG22	1.84	0.58
6:T:2158:LEU:HD12	6:T:2158:LEU:N	2.19	0.58
6:T:2228:GLU:N	6:T:2228:GLU:OE1	2.36	0.58
2:B:14:VAL:HG11	4:E:91:LEU:HD13	1.84	0.58
2:B:262:LEU:O	2:B:282:ASN:ND2	2.37	0.58
2:B:397:ASP:OD1	2:B:398:VAL:N	2.30	0.58
5:F:556:SER:OG	6:T:3519:THR:OG1	2.22	0.58
6:T:1216:ILE:HD11	6:T:1237:LEU:HD23	1.84	0.58
6:T:1372:GLU:OE2	6:T:1432:GLN:NE2	2.37	0.58
6:T:1750:PHE:O	6:T:1750:PHE:HD1	1.87	0.58
3:D:78:ILE:HG13	3:D:79:ARG:H	1.68	0.57
6:T:1562:LEU:HG	6:T:1563:PRO:HD2	1.86	0.57
6:T:2460:TRP:HD1	6:T:2462:PHE:CD1	2.21	0.57
6:T:2811:GLN:HE21	6:T:2814:ARG:HD3	1.69	0.57
6:T:3131:TRP:HD1	6:T:3163:TYR:CZ	2.22	0.57
6:T:126:PHE:CZ	6:T:130:LYS:HD3	2.38	0.57
6:T:1281:GLY:HA2	6:T:1285:LEU:HB2	1.86	0.57
6:T:1617:LEU:HB2	6:T:1620:LEU:HB3	1.86	0.57
6:T:2218:LYS:HG3	6:T:2218:LYS:O	2.03	0.57
6:T:851:LEU:HA	6:T:854:GLU:HB3	1.86	0.57
6:T:1173:GLU:OE1	6:T:1174:LYS:NZ	2.37	0.57
6:T:1234:GLN:NE2	6:T:1271:THR:OG1	2.37	0.57
6:T:1821:LEU:HG	6:T:1821:LEU:O	2.02	0.57
1:A:103:VAL:HG12	1:A:129:VAL:HG11	1.86	0.57
4:E:82:GLU:HG3	4:E:92:ARG:HG2	1.85	0.57
6:T:10:PHE:HA	6:T:30:GLU:HG3	1.86	0.57
6:T:19:ALA:O	6:T:23:SER:N	2.37	0.57
6:T:1486:LEU:HD23	6:T:1489:LEU:HD12	1.86	0.57
6:T:2240:THR:HG23	6:T:2259:LEU:HD22	1.85	0.57
6:T:2357:ARG:O	6:T:2360:ILE:HG22	2.05	0.57
6:T:2459:ASN:HD21	6:T:2468:TRP:NE1	2.02	0.57
6:T:3060:TRP:HD1	6:T:3084:CYS:SG	2.27	0.57
2:B:231:ASP:OD1	2:B:235:ASN:ND2	2.37	0.57
6:T:832:LYS:HG3	6:T:833:PRO:HD3	1.87	0.57
6:T:1490:SER:HA	6:T:1521:LYS:HD2	1.86	0.57
6:T:1930:LEU:HB3	6:T:1946:LEU:HD21	1.85	0.57
6:T:25:TYR:O	6:T:29:SER:OG	2.21	0.57
6:T:480:ARG:HD3	6:T:1760:TYR:CG	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:698:PHE:O	6:T:702:ILE:HG22	2.04	0.57
6:T:2432:ARG:HD3	6:T:2550:TYR:CZ	2.38	0.57
6:T:80:LEU:HD22	6:T:120:LYS:HB3	1.87	0.57
6:T:612:THR:HB	6:T:1532:VAL:HG11	1.86	0.57
6:T:751:LEU:HB2	6:T:808:TYR:CZ	2.40	0.57
6:T:1454:GLU:H	6:T:1454:GLU:CD	2.12	0.57
6:T:1510:LEU:HD23	6:T:1513:TYR:HE1	1.70	0.57
6:T:1949:LEU:HD23	6:T:1949:LEU:O	2.03	0.57
2:B:126:GLU:O	2:B:130:GLU:HB3	2.05	0.57
2:B:130:GLU:O	2:B:133:GLN:NE2	2.38	0.57
6:T:690:PHE:HA	6:T:693:MET:HE3	1.86	0.57
6:T:2322:VAL:HG23	6:T:2322:VAL:O	2.05	0.57
6:T:2621:HIS:ND1	6:T:2622:LEU:HG	2.20	0.57
6:T:3202:ARG:O	6:T:3205:TRP:NE1	2.36	0.57
3:D:597:PHE:CD1	5:F:639:ARG:HB2	2.40	0.57
3:D:645:ARG:O	3:D:736:ARG:NH2	2.33	0.57
6:T:1543:LEU:HD12	6:T:1549:THR:HG21	1.86	0.57
6:T:1699:LEU:HD23	6:T:1699:LEU:C	2.29	0.57
6:T:2209:VAL:HA	6:T:2212:VAL:HG13	1.87	0.57
6:T:2481:ASN:OD1	6:T:2482:ARG:N	2.38	0.57
6:T:507:ILE:HG13	6:T:508:GLN:HG2	1.86	0.57
6:T:1036:PRO:HG2	6:T:1039:TYR:HB2	1.87	0.57
6:T:1962:THR:N	6:T:1963:PRO:HD2	2.20	0.57
6:T:3255:ASP:OD1	6:T:3256:GLY:N	2.38	0.57
6:T:146:GLN:OE1	6:T:150:ASN:ND2	2.38	0.56
6:T:892:ASP:OD1	6:T:892:ASP:N	2.38	0.56
6:T:2426:VAL:HG13	6:T:2428:ASP:H	1.70	0.56
3:D:354:GLN:OE1	4:E:182:ARG:NH1	2.38	0.56
6:T:985:MET:HG2	6:T:2570:SER:HB2	1.88	0.56
1:A:363:ASP:OD1	4:E:76:SER:N	2.24	0.56
3:D:675:HIS:NE2	6:T:2622:LEU:HB2	2.20	0.56
4:E:199:GLU:OE1	4:E:199:GLU:N	2.30	0.56
6:T:240:GLN:O	6:T:244:THR:HG23	2.05	0.56
6:T:352:ARG:HD3	6:T:394:THR:HG22	1.88	0.56
6:T:942:SER:O	6:T:946:VAL:HG23	2.05	0.56
6:T:1379:GLN:O	6:T:1383:VAL:HG23	2.05	0.56
6:T:2036:LEU:HD23	6:T:2123:ILE:HD12	1.87	0.56
6:T:2847:GLN:NE2	6:T:2851:GLU:OE2	2.39	0.56
6:T:2680:ARG:HE	6:T:2689:ASN:ND2	2.03	0.56
2:B:222:ASP:N	2:B:222:ASP:OD1	2.38	0.56
3:D:585:ILE:HG22	3:D:587:LYS:HZ1	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:586:SER:C	3:D:587:LYS:HZ2	2.12	0.56
5:F:627:LEU:HD13	5:F:629:ILE:HG12	1.87	0.56
6:T:80:LEU:O	6:T:84:ASN:ND2	2.39	0.56
6:T:2332:PHE:O	6:T:2336:VAL:HG23	2.06	0.56
6:T:422:LEU:HD12	6:T:474:ARG:HG2	1.87	0.56
6:T:1426:GLU:OE1	6:T:1426:GLU:N	2.38	0.56
6:T:2775:ALA:O	6:T:2778:GLN:NE2	2.38	0.56
3:D:643:GLN:CD	3:D:643:GLN:H	2.14	0.56
6:T:99:VAL:HG21	6:T:125:LEU:HD12	1.87	0.56
6:T:755:ASP:OD1	6:T:758:THR:HG22	2.05	0.56
6:T:808:TYR:O	6:T:812:ILE:HG12	2.05	0.56
6:T:1205:THR:O	6:T:1208:ASN:N	2.39	0.56
6:T:2329:ARG:O	6:T:2333:LEU:HG	2.06	0.56
3:D:272:LEU:HD11	3:D:566:TYR:HE1	1.71	0.56
3:D:292:TYR:O	3:D:296:THR:HG23	2.05	0.56
3:D:549:VAL:HG23	3:D:550:ASP:H	1.71	0.56
6:T:31:LEU:HD22	6:T:82:ILE:HG12	1.87	0.56
6:T:1271:THR:HG23	6:T:1272:PHE:HD1	1.70	0.56
6:T:2188:GLN:HE21	6:T:2192:GLU:HB3	1.70	0.56
6:T:3155:ILE:HG22	6:T:3159:ILE:HD11	1.87	0.56
6:T:3729:SER:OG	6:T:3732:ASN:OD1	2.23	0.56
6:T:434:MET:O	6:T:438:LEU:HG	2.05	0.56
6:T:1354:VAL:O	6:T:1358:THR:HG23	2.06	0.56
6:T:2206:LEU:HD12	6:T:2206:LEU:C	2.31	0.56
6:T:2279:MET:HA	6:T:2279:MET:HE3	1.87	0.56
6:T:3384:THR:HG23	6:T:3385:HIS:HD2	1.71	0.56
2:B:287:GLY:HA2	2:B:290:GLU:HB3	1.87	0.56
6:T:834:ILE:H	6:T:834:ILE:HD12	1.71	0.56
6:T:1110:PHE:HB3	6:T:1145:ILE:HD13	1.88	0.56
6:T:2182:GLU:H	6:T:2182:GLU:CD	2.13	0.56
6:T:2236:ILE:HB	6:T:2259:LEU:HD21	1.87	0.56
1:A:168:GLY:HA3	3:D:384:CYS:HB3	1.87	0.55
2:B:21:PRO:HB2	2:B:75:ILE:HG13	1.88	0.55
6:T:327:ASP:HA	6:T:330:ILE:HG22	1.88	0.55
6:T:3436:THR:HG23	6:T:3441:ILE:HD13	1.86	0.55
6:T:2350:ARG:HA	6:T:2353:VAL:HG22	1.87	0.55
1:A:39:ARG:NH2	1:A:62:ARG:O	2.40	0.55
1:A:117:GLU:OE1	4:E:94:TRP:NE1	2.40	0.55
2:B:210:LYS:N	2:B:217:ILE:O	2.39	0.55
3:D:595:ASN:OD1	3:D:596:GLY:N	2.31	0.55
5:F:577:TYR:O	5:F:580:HIS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:580:HIS:CG	5:F:581:LEU:N	2.74	0.55
6:T:3041:GLN:O	6:T:3045:THR:HG23	2.06	0.55
6:T:826:ASN:OD1	6:T:827:LEU:N	2.38	0.55
6:T:1673:PHE:HZ	6:T:1692:ILE:HG22	1.71	0.55
6:T:1740:GLN:HE22	6:T:1781:ASN:HB2	1.71	0.55
6:T:1895:LYS:H	6:T:1895:LYS:HD2	1.72	0.55
6:T:2482:ARG:HH21	6:T:2539:SER:HA	1.72	0.55
6:T:2892:TRP:CD2	6:T:3437:ARG:HG2	2.42	0.55
3:D:575:LYS:HE2	3:D:577:ASP:HB3	1.88	0.55
6:T:410:GLU:O	6:T:414:THR:HG23	2.07	0.55
6:T:796:LEU:HD13	6:T:838:LEU:HD23	1.88	0.55
6:T:972:LEU:HD23	6:T:998:GLN:HG3	1.89	0.55
6:T:1702:THR:HA	6:T:1705:THR:HG22	1.87	0.55
1:A:358:SER:OG	1:A:361:GLU:N	2.33	0.55
4:E:274:GLU:HB3	4:E:275:ARG:NH2	2.22	0.55
5:F:581:LEU:HG	5:F:615:LYS:HB2	1.88	0.55
6:T:1641:GLU:HG2	6:T:1676:MET:HE2	1.89	0.55
6:T:1864:LEU:HD11	6:T:1893:PHE:HZ	1.71	0.55
6:T:2100:LEU:HD21	6:T:2121:ILE:HD13	1.88	0.55
6:T:3154:HIS:O	6:T:3158:ARG:NH1	2.39	0.55
6:T:3416:GLU:HG3	6:T:3420:PHE:CE2	2.42	0.55
6:T:3717:THR:O	6:T:3720:ILE:N	2.40	0.55
2:B:272:SER:OG	2:B:276:GLU:N	2.39	0.55
6:T:572:LEU:CA	6:T:1940:TYR:CE2	2.90	0.55
6:T:1331:GLN:HA	6:T:1334:LEU:HG	1.88	0.55
1:A:51:ASP:OD1	1:A:51:ASP:N	2.39	0.55
1:A:188:TYR:HE2	1:A:257:ALA:HA	1.71	0.55
3:D:762:GLU:HA	3:D:765:ARG:HH11	1.71	0.55
6:T:339:GLU:HB3	6:T:1897:GLU:HB3	1.88	0.55
6:T:1030:LYS:HA	6:T:2534:CYS:SG	2.47	0.55
6:T:3564:ILE:HG13	6:T:3565:ASN:H	1.71	0.55
2:B:103:ASN:HA	2:B:106:ILE:HD12	1.89	0.55
3:D:637:PRO:HG2	3:D:723:TRP:NE1	2.21	0.55
6:T:1198:ILE:HD11	6:T:1237:LEU:HG	1.89	0.55
6:T:1532:VAL:HG22	6:T:1583:LYS:HE2	1.89	0.55
6:T:2741:GLN:HG3	6:T:2742:HIS:H	1.72	0.55
6:T:3082:ILE:HD12	6:T:3107:LEU:HB3	1.89	0.55
1:A:58:ALA:HB1	1:A:67:LEU:HD21	1.88	0.54
1:A:152:VAL:HG13	1:A:298:VAL:HG12	1.88	0.54
6:T:337:PRO:O	6:T:344:ARG:NH2	2.40	0.54
6:T:382:THR:HG23	6:T:1900:LEU:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:590:LEU:O	6:T:594:LEU:HG	2.07	0.54
6:T:1132:ASP:HA	6:T:3320:ARG:HH22	1.71	0.54
6:T:1146:LEU:HD13	6:T:1193:LEU:HD22	1.88	0.54
6:T:2118:LEU:HD23	6:T:2118:LEU:O	2.08	0.54
6:T:2320:LEU:CD1	6:T:2356:SER:N	2.60	0.54
1:A:110:MET:SD	2:B:37:GLN:NE2	2.81	0.54
2:B:396:SER:OG	2:B:397:ASP:N	2.40	0.54
2:B:480:VAL:HA	2:B:483:LEU:HD12	1.88	0.54
6:T:1159:GLU:O	6:T:1163:VAL:HG23	2.07	0.54
6:T:1485:LEU:HB3	6:T:1503:LEU:HD21	1.89	0.54
6:T:1912:PHE:CD1	6:T:1912:PHE:C	2.85	0.54
6:T:2311:LEU:C	6:T:2311:LEU:HD12	2.33	0.54
6:T:3034:ARG:NH2	6:T:3036:TYR:OH	2.35	0.54
1:A:4:GLU:OE1	1:A:5:VAL:HG22	2.07	0.54
1:A:136:ILE:HG23	1:A:139:VAL:HG12	1.90	0.54
3:D:66:ASP:HB3	3:D:537:LYS:HE3	1.89	0.54
6:T:709:VAL:O	6:T:713:MET:HG3	2.07	0.54
6:T:1284:VAL:HG13	6:T:1285:LEU:HD22	1.89	0.54
6:T:1487:MET:CA	6:T:1487:MET:CE	2.85	0.54
6:T:1506:LEU:HD12	6:T:1506:LEU:O	2.07	0.54
6:T:1750:PHE:C	6:T:1750:PHE:CD1	2.85	0.54
6:T:3435:GLU:OE2	6:T:3439:ARG:NH1	2.37	0.54
6:T:769:SER:O	6:T:773:VAL:HG23	2.07	0.54
6:T:2748:GLU:OE1	6:T:2748:GLU:N	2.31	0.54
6:T:2847:GLN:O	6:T:2851:GLU:HG2	2.08	0.54
6:T:639:HIS:CE1	6:T:643:ILE:HD11	2.43	0.54
6:T:769:SER:O	6:T:772:SER:OG	2.17	0.54
6:T:934:PRO:HG3	6:T:2826:ILE:HA	1.90	0.54
6:T:1449:LEU:CD2	6:T:1484:PRO:CG	2.82	0.54
6:T:1859:LEU:N	6:T:1859:LEU:HD23	2.22	0.54
6:T:1915:LYS:CA	6:T:1915:LYS:CE	2.86	0.54
6:T:2174:ASN:HB3	6:T:2175:LYS:HE2	1.90	0.54
6:T:3237:PHE:CD2	6:T:3405:VAL:HG21	2.43	0.54
3:D:33:ILE:HG13	3:D:36:ARG:CZ	2.38	0.54
3:D:586:SER:O	3:D:587:LYS:NZ	2.37	0.54
4:E:169:ILE:HA	4:E:196:ARG:HH22	1.73	0.54
6:T:3566:ASN:O	6:T:3567:ARG:NE	2.36	0.54
1:A:221:LEU:O	1:A:315:LYS:NZ	2.36	0.54
6:T:10:PHE:HB2	6:T:13:ARG:HE	1.72	0.54
6:T:339:GLU:CD	6:T:1897:GLU:CB	2.80	0.54
6:T:1004:LEU:HD21	6:T:1089:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2411:GLU:OE1	6:T:2411:GLU:N	2.41	0.54
6:T:2590:PRO:HD2	6:T:2592:HIS:O	2.07	0.54
6:T:3680:ARG:HD2	6:T:3683:ILE:HG21	1.90	0.54
4:E:298:GLN:NE2	4:E:301:SER:H	2.04	0.54
6:T:480:ARG:CZ	6:T:1760:TYR:CD1	2.91	0.54
6:T:2278:LEU:HD12	6:T:2278:LEU:O	2.07	0.54
6:T:2691:GLY:HA3	6:T:2707:TYR:CE1	2.43	0.54
6:T:15:ARG:HH22	6:T:27:THR:HB	1.71	0.54
6:T:1420:ALA:CB	6:T:1462:ALA:HB1	2.38	0.54
6:T:2189:ASN:HD22	6:T:2189:ASN:N	2.04	0.54
6:T:2191:LEU:HD12	6:T:2194:CYS:HB2	1.90	0.54
6:T:2210:LEU:HD11	6:T:2258:THR:HB	1.88	0.54
3:D:308:LYS:NZ	6:T:2689:ASN:OD1	2.41	0.54
6:T:792:ILE:O	6:T:795:SER:OG	2.19	0.54
6:T:1107:LEU:HD22	6:T:1171:ILE:HD11	1.88	0.54
6:T:1568:MET:HE1	6:T:1572:ASP:HB2	1.89	0.54
6:T:1985:LEU:HA	6:T:1988:PHE:CE2	2.43	0.54
6:T:2206:LEU:HD23	6:T:2255:ALA:HA	1.90	0.54
6:T:3405:VAL:HG12	6:T:3457:ILE:HG22	1.90	0.54
6:T:786:PRO:O	6:T:787:HIS:ND1	2.40	0.53
6:T:846:ILE:HG12	6:T:848:THR:O	2.08	0.53
6:T:1776:LYS:HE2	6:T:1778:LYS:HE3	1.89	0.53
6:T:2031:LEU:HD12	6:T:2031:LEU:C	2.32	0.53
6:T:2862:LEU:HD11	6:T:2915:ALA:HB3	1.90	0.53
6:T:480:ARG:NH1	6:T:1760:TYR:CG	2.73	0.53
6:T:849:ALA:C	6:T:851:LEU:H	2.14	0.53
6:T:3551:GLN:NE2	6:T:3580:ASN:OD1	2.41	0.53
1:A:160:THR:HG23	1:A:178:ILE:HB	1.89	0.53
2:B:141:PRO:O	2:B:144:THR:OG1	2.23	0.53
6:T:678:ASP:O	6:T:682:LEU:HG	2.08	0.53
6:T:823:ARG:O	6:T:826:ASN:N	2.24	0.53
6:T:1444:PHE:O	6:T:1448:MET:HG2	2.08	0.53
6:T:1752:PHE:CE1	6:T:1796:LEU:HD21	2.44	0.53
6:T:1776:LYS:HZ3	6:T:1778:LYS:HG3	1.73	0.53
6:T:1801:PHE:CE1	6:T:1859:LEU:HB2	2.43	0.53
6:T:2365:ILE:HG13	6:T:2366:PHE:N	2.23	0.53
6:T:3240:THR:HG23	6:T:3242:ASP:H	1.73	0.53
6:T:3466:THR:HG22	6:T:3573:HIS:CD2	2.43	0.53
1:A:99:GLU:H	1:A:99:GLU:CD	2.14	0.53
6:T:402:ILE:HG13	6:T:403:ARG:H	1.73	0.53
6:T:1300:ASN:ND2	6:T:1303:VAL:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1522:LEU:C	6:T:1522:LEU:HD23	2.34	0.53
6:T:2452:TYR:OH	6:T:2575:GLU:OE2	2.25	0.53
6:T:2470:ASN:O	6:T:2474:GLN:HG2	2.09	0.53
6:T:2701:ASP:N	6:T:2701:ASP:OD1	2.39	0.53
1:A:207:GLU:HG2	1:A:210:ARG:HH21	1.72	0.53
2:B:183:ASN:HD21	2:B:185:ILE:HB	1.73	0.53
3:D:743:VAL:HG11	3:D:747:SER:H	1.72	0.53
6:T:440:LEU:O	6:T:443:VAL:HG22	2.07	0.53
6:T:1097:ASP:OD1	6:T:1097:ASP:N	2.41	0.53
6:T:1340:LYS:HE2	6:T:1345:LEU:HD13	1.90	0.53
6:T:1825:LEU:HD23	6:T:1875:ASP:HB2	1.90	0.53
6:T:2708:GLU:OE2	6:T:2733:TRP:NE1	2.41	0.53
6:T:3551:GLN:O	6:T:3554:SER:OG	2.21	0.53
1:A:200:PHE:HA	1:A:205:GLU:HG3	1.90	0.53
1:A:239:SER:HA	1:A:249:THR:HA	1.91	0.53
2:B:144:THR:O	2:B:147:SER:OG	2.22	0.53
3:D:51:GLN:HE21	3:D:54:GLU:CD	2.16	0.53
4:E:281:LEU:HD13	6:T:2685:TYR:C	2.34	0.53
5:F:540:ASP:OD1	5:F:545:PRO:HD3	2.09	0.53
6:T:2862:LEU:HD12	6:T:2912:ILE:HG13	1.90	0.53
4:E:169:ILE:HD13	4:E:204:LYS:HE2	1.90	0.53
6:T:1899:THR:HA	6:T:1902:LYS:HE2	1.90	0.53
6:T:2486:LEU:HD23	6:T:2536:ILE:HG22	1.91	0.53
1:A:39:ARG:NH2	1:A:65:LEU:O	2.42	0.53
6:T:8:GLU:OE2	6:T:9:GLN:NE2	2.41	0.53
6:T:37:LEU:HD12	6:T:2009:HIS:CD2	2.44	0.53
6:T:741:LEU:HD23	6:T:787:HIS:CE1	2.43	0.53
6:T:1312:HIS:O	6:T:1315:SER:OG	2.23	0.53
6:T:1438:ILE:HD12	6:T:1473:LEU:HG	1.91	0.53
6:T:2225:ILE:HG22	6:T:2226:ILE:HG23	1.90	0.53
6:T:2245:GLN:HA	6:T:2245:GLN:HE21	1.71	0.53
6:T:2549:PHE:CD1	6:T:2556:ILE:HG22	2.44	0.53
6:T:2898:TRP:CE3	6:T:2953:VAL:HG11	2.43	0.53
6:T:15:ARG:NH2	6:T:18:ASP:OD1	2.43	0.53
6:T:76:ARG:HB3	6:T:117:LEU:HD11	1.90	0.53
6:T:479:ASN:ND2	6:T:640:GLU:O	2.42	0.53
6:T:2394:PHE:O	6:T:2397:ILE:HG12	2.08	0.53
6:T:3715:VAL:O	6:T:3716:THR:OG1	2.23	0.53
1:A:49:GLN:NE2	1:A:50:LYS:O	2.42	0.52
1:A:100:GLU:HG2	1:A:101:HIS:CE1	2.45	0.52
6:T:613:VAL:HA	6:T:1536:ASP:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1205:THR:HG22	6:T:1207:TYR:HB2	1.92	0.52
6:T:3302:ASP:C	6:T:3304:LYS:H	2.17	0.52
2:B:83:TRP:CD1	2:B:123:LYS:HZ3	2.28	0.52
3:D:30:ASP:O	3:D:33:ILE:HG22	2.09	0.52
3:D:349:ILE:HG13	3:D:351:PRO:HD3	1.91	0.52
3:D:583:ILE:HB	3:D:584:PRO:HD3	1.91	0.52
6:T:365:PRO:HG3	6:T:398:PHE:CZ	2.45	0.52
6:T:1382:ILE:O	6:T:1412:ARG:NH2	2.34	0.52
6:T:1996:PHE:C	6:T:1996:PHE:CD2	2.87	0.52
6:T:3054:ALA:HB3	6:T:3092:TYR:HB2	1.91	0.52
2:B:48:THR:OG1	2:B:68:ASP:OD1	2.27	0.52
3:D:683:SER:OG	3:D:684:TYR:N	2.40	0.52
6:T:1359:PHE:O	6:T:1363:LEU:HG	2.10	0.52
6:T:1883:LYS:HB3	6:T:1912:PHE:CZ	2.43	0.52
6:T:3112:ASP:OD1	6:T:3112:ASP:N	2.43	0.52
6:T:59:LEU:HD11	6:T:83:PHE:CE2	2.45	0.52
6:T:75:LEU:O	6:T:79:MET:HG3	2.10	0.52
6:T:467:ILE:O	6:T:470:SER:OG	2.18	0.52
6:T:640:GLU:HA	6:T:643:ILE:HD12	1.92	0.52
6:T:1281:GLY:O	6:T:1286:GLU:HB2	2.08	0.52
6:T:1742:PRO:HA	6:T:1745:LEU:HD12	1.90	0.52
6:T:2783:VAL:HG12	6:T:2791:ARG:HE	1.73	0.52
6:T:3106:TRP:HE3	6:T:3107:LEU:HD22	1.75	0.52
1:A:181:ALA:N	1:A:184:ASP:OD2	2.43	0.52
6:T:473:ASN:O	6:T:477:THR:HG23	2.10	0.52
6:T:572:LEU:CA	6:T:1940:TYR:HD2	2.21	0.52
6:T:1040:THR:OG1	6:T:1041:GLU:OE1	2.24	0.52
6:T:1513:TYR:O	6:T:1513:TYR:HD1	1.92	0.52
6:T:1830:LYS:HA	6:T:1832:LYS:HE3	1.91	0.52
3:D:533:GLU:OE2	3:D:552:LEU:N	2.43	0.52
6:T:496:LYS:O	6:T:499:LYS:HG3	2.09	0.52
6:T:507:ILE:HG13	6:T:508:GLN:N	2.24	0.52
6:T:1906:TYR:HA	6:T:1909:THR:HG22	1.91	0.52
6:T:326:PRO:HG2	6:T:367:LEU:HD13	1.92	0.52
6:T:697:THR:O	6:T:701:ILE:HG12	2.10	0.52
6:T:1950:THR:HG1	6:T:1951:PRO:HD3	1.74	0.52
6:T:3240:THR:HG23	6:T:3242:ASP:N	2.25	0.52
3:D:265:ALA:O	3:D:266:LEU:HG	2.10	0.52
3:D:682:TYR:HD1	6:T:2667:VAL:HG13	1.74	0.52
6:T:1298:ASN:OD1	6:T:1299:ALA:N	2.39	0.52
6:T:1301:PRO:HA	6:T:1304:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1441:LEU:HD23	6:T:1444:PHE:HD2	1.74	0.52
6:T:2271:ILE:HG13	6:T:2273:PRO:HD2	1.92	0.52
6:T:2519:LEU:H	6:T:2519:LEU:HD12	1.75	0.52
6:T:2959:MET:O	6:T:2962:VAL:HG12	2.10	0.52
6:T:2966:GLN:HA	6:T:2969:ARG:HH22	1.75	0.52
1:A:218:TYR:HA	1:A:307:PRO:HD2	1.90	0.52
2:B:261:GLU:O	2:B:264:SER:OG	2.25	0.52
6:T:349:HIS:HD2	6:T:352:ARG:HH12	1.58	0.52
6:T:1178:ILE:HG23	6:T:1179:TYR:CD1	2.45	0.52
6:T:1509:LEU:N	6:T:1509:LEU:CD2	2.73	0.52
6:T:1611:PHE:HB2	6:T:1624:MET:HE1	1.91	0.52
6:T:1651:TYR:CE2	6:T:1669:MET:HB3	2.45	0.52
6:T:2359:TRP:O	6:T:2372:LYS:NZ	2.39	0.52
3:D:628:ASN:H	6:T:2591:TYR:HE2	1.57	0.52
6:T:473:ASN:HA	6:T:476:LYS:HE2	1.92	0.52
6:T:1673:PHE:CE2	6:T:1695:LEU:HD11	2.45	0.52
6:T:2195:ILE:HG23	6:T:2239:LEU:HD22	1.91	0.52
6:T:2325:LEU:HD11	6:T:2328:SER:C	2.35	0.52
6:T:2420:PHE:HE2	6:T:2439:LEU:HD13	1.75	0.52
2:B:181:ARG:NH2	2:B:395:SER:OG	2.43	0.51
3:D:42:GLU:O	3:D:46:VAL:HG12	2.10	0.51
3:D:59:ASN:OD1	3:D:60:LYS:N	2.43	0.51
6:T:72:GLU:HB2	6:T:76:ARG:HH21	1.75	0.51
6:T:979:ASP:OD1	6:T:979:ASP:N	2.43	0.51
6:T:1510:LEU:HD11	6:T:1563:PRO:HD3	1.92	0.51
6:T:1559:PHE:HB3	6:T:1599:TYR:CD1	2.45	0.51
6:T:1673:PHE:CZ	6:T:1692:ILE:HG22	2.45	0.51
6:T:2687:GLU:OE1	6:T:2687:GLU:N	2.23	0.51
1:A:13:GLY:HA2	1:A:137:GLN:HE22	1.75	0.51
6:T:58:GLN:HG2	6:T:79:MET:HE2	1.91	0.51
6:T:222:LYS:HZ1	6:T:234:LEU:HD22	1.75	0.51
6:T:381:PHE:CE1	6:T:1856:HIS:CE1	2.98	0.51
6:T:752:GLY:HA3	6:T:802:ALA:HB1	1.92	0.51
6:T:856:GLU:HB3	6:T:890:TYR:CE1	2.45	0.51
6:T:984:GLY:HA3	6:T:2447:ILE:HG22	1.91	0.51
1:A:286:ASP:OD1	1:A:287:VAL:N	2.40	0.51
2:B:253:LYS:HE3	2:B:257:GLU:HG3	1.93	0.51
6:T:2180:ILE:O	6:T:2180:ILE:HG13	2.10	0.51
6:T:3087:GLN:HG2	6:T:3124:PHE:HE1	1.75	0.51
2:B:23:SER:N	7:B:501:ATP:O3G	2.43	0.51
3:D:751:GLY:HA2	3:D:755:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:560:VAL:O	5:F:562:PHE:N	2.44	0.51
6:T:1939:ARG:NH1	6:T:1939:ARG:CB	2.73	0.51
6:T:2621:HIS:CE1	6:T:2657:ALA:HB1	2.45	0.51
6:T:2650:ASP:OD1	6:T:2650:ASP:N	2.44	0.51
6:T:3172:ARG:NH2	6:T:3227:GLU:OE1	2.43	0.51
2:B:21:PRO:HA	2:B:26:THR:HG23	1.92	0.51
6:T:1353:ASN:O	6:T:1357:ILE:HG13	2.11	0.51
6:T:1601:ASN:HD22	6:T:1601:ASN:N	2.07	0.51
6:T:1941:LEU:HD12	6:T:1941:LEU:C	2.35	0.51
6:T:2143:PHE:CZ	6:T:2170:VAL:HG11	2.45	0.51
6:T:2164:ALA:HA	6:T:2167:VAL:HG22	1.92	0.51
6:T:2214:MET:C	6:T:2214:MET:SD	2.94	0.51
6:T:2669:LEU:HD22	6:T:2836:THR:HG21	1.91	0.51
6:T:3156:LEU:HA	6:T:3159:ILE:HD12	1.93	0.51
6:T:3493:LEU:HG	6:T:3509:LEU:HD21	1.92	0.51
1:A:70:PRO:O	1:A:77:THR:N	2.43	0.51
1:A:372:HIS:HE1	5:F:644:ARG:CZ	2.24	0.51
6:T:443:VAL:HA	6:T:446:ILE:HD12	1.92	0.51
6:T:1045:THR:HG21	6:T:2510:MET:HA	1.93	0.51
6:T:1625:CYS:HA	6:T:1628:VAL:HG12	1.93	0.51
6:T:1867:LEU:C	6:T:1867:LEU:HD12	2.36	0.51
6:T:3736:THR:HG21	6:T:3740:PHE:HD2	1.75	0.51
1:A:275:ASP:N	1:A:275:ASP:OD1	2.40	0.51
1:A:311:GLU:OE1	1:A:311:GLU:N	2.43	0.51
3:D:272:LEU:HD11	3:D:566:TYR:CE1	2.46	0.51
6:T:381:PHE:O	6:T:385:GLU:N	2.41	0.51
6:T:1511:ILE:HG23	6:T:1511:ILE:O	2.09	0.51
6:T:3203:GLN:HG3	6:T:3207:TYR:HE2	1.75	0.51
1:A:151:ILE:HA	1:A:164:PRO:HA	1.91	0.51
3:D:633:PRO:HB3	3:D:697:PHE:CZ	2.46	0.51
4:E:98:SER:O	4:E:102:ILE:HG12	2.10	0.51
6:T:80:LEU:HD13	6:T:120:LYS:HG2	1.93	0.51
6:T:519:ARG:HA	6:T:522:LEU:HD12	1.92	0.51
6:T:1131:ILE:HG23	6:T:3320:ARG:HG2	1.93	0.51
6:T:1132:ASP:HA	6:T:3320:ARG:NH2	2.26	0.51
6:T:1159:GLU:OE1	6:T:1159:GLU:N	2.39	0.51
4:E:294:TYR:HB3	6:T:2712:VAL:HG11	1.93	0.51
6:T:1848:ILE:HB	6:T:1852:ASP:HB2	1.93	0.51
6:T:2271:ILE:HG23	6:T:2274:LEU:HB2	1.93	0.51
1:A:82:MET:HA	1:A:85:ILE:HD12	1.93	0.51
2:B:116:ASN:OD1	2:B:117:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:ILE:HG23	5:F:577:TYR:OH	2.11	0.51
3:D:347:ARG:HD2	3:D:585:ILE:HD11	1.92	0.51
6:T:381:PHE:N	6:T:1858:ASP:OD1	2.43	0.51
6:T:477:THR:O	6:T:481:GLN:HG2	2.10	0.51
6:T:481:GLN:N	6:T:1760:TYR:HH	2.08	0.51
6:T:1062:ASP:OD1	6:T:1062:ASP:N	2.38	0.51
6:T:1157:ILE:O	6:T:1160:VAL:HG22	2.10	0.51
6:T:1423:LEU:HD12	6:T:1466:SER:OG	2.11	0.51
6:T:3304:LYS:N	6:T:3305:PRO:HD2	2.26	0.51
1:A:242:LEU:HD13	1:A:246:GLN:HB3	1.93	0.50
2:B:41:PRO:HD3	2:B:59:GLU:HB2	1.94	0.50
3:D:621:MET:HE3	3:D:625:ASN:HB3	1.93	0.50
3:D:762:GLU:HA	3:D:765:ARG:HD3	1.93	0.50
6:T:379:ASN:OD1	6:T:1856:HIS:HA	2.12	0.50
6:T:570:LEU:HD23	6:T:570:LEU:H	1.77	0.50
6:T:3412:HIS:CD2	6:T:3587:LEU:HD21	2.46	0.50
3:D:293:MET:O	3:D:296:THR:OG1	2.23	0.50
5:F:520:VAL:O	5:F:524:MET:HG3	2.11	0.50
6:T:611:TYR:OH	6:T:1584:LEU:C	2.54	0.50
6:T:858:TYR:HA	6:T:861:LEU:HD12	1.92	0.50
6:T:1405:SER:OG	6:T:1406:GLU:OE1	2.27	0.50
6:T:1516:VAL:HG11	6:T:1562:LEU:HD21	1.93	0.50
6:T:2197:SER:HA	6:T:2200:HIS:CE1	2.47	0.50
4:E:218:PRO:HA	4:E:223:LEU:HD12	1.93	0.50
6:T:24:ARG:NH2	6:T:70:SER:O	2.45	0.50
6:T:711:GLU:O	6:T:714:LEU:HB2	2.11	0.50
6:T:757:ASN:O	6:T:761:VAL:HG23	2.11	0.50
6:T:942:SER:OG	6:T:943:HIS:ND1	2.44	0.50
6:T:1655:ILE:N	6:T:1656:PRO:HD2	2.26	0.50
1:A:164:PRO:HG2	1:A:171:LEU:HD12	1.94	0.50
2:B:247:CYS:HB2	2:B:417:ILE:HD12	1.93	0.50
6:T:713:MET:HE3	6:T:719:LEU:HB2	1.93	0.50
6:T:918:GLU:HA	6:T:921:ILE:HG13	1.94	0.50
6:T:1641:GLU:HB3	6:T:1684:TRP:CZ2	2.45	0.50
6:T:3613:ILE:HG22	6:T:3614:PHE:H	1.77	0.50
3:D:609:GLU:O	3:D:611:SER:N	2.44	0.50
3:D:619:ARG:HD2	3:D:619:ARG:N	2.27	0.50
6:T:598:ILE:HD11	6:T:689:MET:HB3	1.93	0.50
6:T:912:TYR:O	6:T:915:PRO:HD2	2.12	0.50
6:T:1449:LEU:HD22	6:T:1484:PRO:CB	2.40	0.50
6:T:1482:LEU:HG	6:T:1482:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2156:ASN:HA	6:T:2159:TYR:CD2	2.46	0.50
6:T:2342:HIS:O	6:T:2385:ARG:NH2	2.29	0.50
6:T:3266:PRO:HA	6:T:3498:ASP:HB3	1.93	0.50
6:T:3413:SER:OG	6:T:3417:GLU:OE2	2.30	0.50
1:A:169:PHE:HZ	3:D:381:VAL:HG22	1.77	0.50
1:A:196:ARG:NH1	1:A:253:GLU:OE2	2.43	0.50
2:B:209:ILE:HA	2:B:218:LYS:HA	1.94	0.50
3:D:684:TYR:CD2	6:T:2757:ASP:HB2	2.46	0.50
4:E:298:GLN:HE22	4:E:301:SER:H	1.59	0.50
6:T:307:TYR:OH	6:T:347:LEU:HB2	2.11	0.50
6:T:434:MET:HA	6:T:437:LYS:HD2	1.94	0.50
6:T:1437:ARG:HA	6:T:1440:ILE:HG22	1.93	0.50
6:T:1570:LEU:HD23	6:T:1570:LEU:O	2.12	0.50
6:T:1977:ASN:HD21	6:T:1983:ASN:HA	1.76	0.50
6:T:2337:ALA:HA	6:T:2340:ILE:HD12	1.93	0.50
6:T:2338:LEU:HG	6:T:2342:HIS:NE2	2.26	0.50
6:T:3426:PHE:HE2	6:T:3561:MET:HE1	1.77	0.50
2:B:43:VAL:HG12	2:B:73:PRO:HA	1.93	0.50
2:B:478:VAL:HG22	2:B:482:ARG:HG2	1.94	0.50
3:D:71:LYS:HA	3:D:74:ILE:HG22	1.93	0.50
6:T:477:THR:HA	6:T:480:ARG:HD2	1.94	0.50
6:T:1115:VAL:HA	6:T:1118:THR:HG22	1.94	0.50
6:T:1210:ARG:HB2	6:T:1256:ILE:HD12	1.93	0.50
6:T:2616:LEU:O	6:T:2617:GLU:HG2	2.11	0.50
6:T:2619:PRO:N	6:T:2620:PRO:HD2	2.26	0.50
6:T:3306:ASP:OD1	6:T:3309:THR:HG22	2.11	0.50
1:A:98:PRO:HA	1:A:101:HIS:HD2	1.76	0.50
5:F:574:ARG:HG2	5:F:574:ARG:O	2.12	0.50
6:T:103:LEU:HD22	6:T:122:LEU:HG	1.93	0.50
1:A:80:ASP:OD1	1:A:81:ASP:N	2.44	0.50
3:D:543:PHE:O	3:D:545:LEU:HG	2.12	0.50
6:T:99:VAL:O	6:T:103:LEU:HG	2.11	0.50
6:T:381:PHE:HE1	6:T:1856:HIS:CE1	2.30	0.50
6:T:2189:ASN:N	6:T:2189:ASN:ND2	2.60	0.50
6:T:2320:LEU:HD13	6:T:2355:MET:HB3	0.54	0.50
6:T:2588:SER:OG	6:T:2589:LYS:N	2.45	0.50
5:F:524:MET:O	5:F:528:LYS:HG2	2.12	0.49
6:T:562:ASP:OD1	6:T:565:ASN:ND2	2.31	0.49
6:T:847:LEU:H	6:T:1207:TYR:HE2	1.59	0.49
6:T:1001:LEU:HD21	6:T:1085:SER:HB2	1.94	0.49
6:T:1102:LEU:HA	6:T:1105:ASN:HD22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1335:SER:OG	6:T:1336:PRO:HD3	2.12	0.49
6:T:1832:LYS:HE2	6:T:1832:LYS:N	2.27	0.49
6:T:1858:ASP:OD1	6:T:1858:ASP:N	2.45	0.49
6:T:2006:ASN:HA	6:T:2009:HIS:CD2	2.47	0.49
6:T:2282:PHE:HE1	6:T:2335:THR:HB	1.77	0.49
6:T:2588:SER:O	6:T:2594:ARG:NH2	2.35	0.49
6:T:2633:TRP:CD1	6:T:2832:PRO:HD3	2.46	0.49
1:A:341:ILE:O	1:A:344:SER:OG	2.29	0.49
2:B:16:ALA:HB2	2:B:107:PRO:HG2	1.94	0.49
4:E:272:LEU:O	4:E:276:GLU:HG2	2.12	0.49
6:T:1650:PHE:C	6:T:1650:PHE:CD2	2.90	0.49
6:T:2138:VAL:HG22	6:T:2142:TYR:CD1	2.48	0.49
6:T:2184:LEU:C	6:T:2184:LEU:CD2	2.86	0.49
6:T:3020:ALA:O	6:T:3024:THR:HG23	2.11	0.49
6:T:624:ARG:O	6:T:1585:ARG:HD2	2.12	0.49
6:T:1378:LEU:HB3	6:T:1415:CYS:SG	2.52	0.49
6:T:1491:ASP:HA	6:T:1525:HIS:CE1	2.48	0.49
6:T:1605:ASN:H	6:T:1606:PRO:CD	2.25	0.49
6:T:1699:LEU:C	6:T:1699:LEU:CD2	2.86	0.49
6:T:1765:PHE:HA	6:T:1768:HIS:CE1	2.46	0.49
3:D:752:HIS:H	3:D:755:LEU:HB3	1.77	0.49
4:E:274:GLU:HB3	4:E:275:ARG:HH22	1.77	0.49
6:T:612:THR:O	6:T:1532:VAL:CG1	2.60	0.49
6:T:789:ASN:HB3	6:T:828:TYR:CE1	2.47	0.49
6:T:1857:HIS:HB3	6:T:1859:LEU:HG	1.94	0.49
6:T:1875:ASP:HB3	6:T:1878:ILE:HG22	1.95	0.49
6:T:2124:LEU:HD23	6:T:2124:LEU:O	2.12	0.49
6:T:2999:LEU:HD23	6:T:3003:LEU:HD23	1.94	0.49
6:T:3441:ILE:HG21	6:T:3648:ILE:HD11	1.94	0.49
5:F:581:LEU:HD21	5:F:613:ARG:HA	1.94	0.49
6:T:137:LEU:HD21	6:T:228:PRO:HG2	1.95	0.49
6:T:796:LEU:O	6:T:800:THR:HG23	2.12	0.49
6:T:1483:LYS:HB3	6:T:1484:PRO:HD3	1.94	0.49
6:T:2361:PHE:HZ	6:T:2400:LYS:HG2	1.78	0.49
6:T:2973:LEU:HD12	6:T:2974:PRO:HD2	1.95	0.49
6:T:34:ILE:HB	6:T:38:LEU:HD11	1.95	0.49
6:T:1419:LEU:O	6:T:1423:LEU:HG	2.12	0.49
6:T:1564:PRO:HA	6:T:1603:PHE:CE1	2.47	0.49
6:T:1748:ILE:HD11	6:T:1789:PHE:HZ	1.78	0.49
6:T:2160:TYR:HA	6:T:2163:ASN:ND2	2.28	0.49
6:T:2602:VAL:HA	6:T:2605:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2708:GLU:O	6:T:2712:VAL:HG23	2.13	0.49
6:T:3460:ASP:HA	6:T:3464:PHE:HZ	1.76	0.49
3:D:39:LYS:HA	6:T:3508:ILE:HG21	1.95	0.49
6:T:72:GLU:O	6:T:76:ARG:HG3	2.12	0.49
6:T:789:ASN:OD1	6:T:790:ASP:N	2.42	0.49
6:T:1546:GLN:HG2	6:T:1549:THR:HG23	1.93	0.49
6:T:1821:LEU:HD11	6:T:1824:TYR:HB2	1.94	0.49
6:T:2143:PHE:HZ	6:T:2170:VAL:HG11	1.76	0.49
6:T:2329:ARG:HG3	6:T:2330:ARG:N	2.28	0.49
6:T:2461:GLU:HA	6:T:2592:HIS:CD2	2.47	0.49
6:T:2626:LEU:HD23	6:T:2626:LEU:O	2.12	0.49
6:T:3422:LEU:HB2	6:T:3666:PHE:HD2	1.78	0.49
6:T:3423:TYR:CD2	6:T:3558:MET:HG2	2.48	0.49
1:A:125:GLU:OE2	4:E:77:PRO:HA	2.13	0.49
2:B:261:GLU:OE1	2:B:261:GLU:N	2.45	0.49
2:B:277:GLU:OE1	2:B:279:VAL:HG23	2.13	0.49
3:D:22:ASP:OD1	3:D:23:ARG:N	2.45	0.49
3:D:379:TYR:CZ	3:D:532:THR:HG21	2.48	0.49
3:D:722:GLN:HA	3:D:725:ILE:HG22	1.95	0.49
6:T:31:LEU:HD23	6:T:35:MET:HE2	1.95	0.49
6:T:129:PHE:HA	6:T:132:ILE:HG12	1.95	0.49
6:T:686:LEU:HA	6:T:689:MET:SD	2.53	0.49
6:T:715:GLU:OE1	6:T:715:GLU:N	2.45	0.49
6:T:1179:TYR:HB2	6:T:1184:ALA:HB2	1.95	0.49
6:T:1463:LEU:C	6:T:1463:LEU:CD2	2.86	0.49
6:T:1776:LYS:HE2	6:T:1778:LYS:CE	2.43	0.49
6:T:1778:LYS:HA	6:T:1781:ASN:ND2	2.28	0.49
6:T:2320:LEU:CD2	6:T:2320:LEU:C	2.86	0.49
6:T:2790:ARG:NH1	6:T:2793:MET:SD	2.86	0.49
1:A:19:ALA:O	1:A:28:ARG:N	2.43	0.49
2:B:242:CYS:HB3	2:B:246:LEU:HD12	1.95	0.49
6:T:129:PHE:HZ	6:T:136:LYS:H	1.59	0.49
6:T:311:ARG:HH21	6:T:315:PRO:HD3	1.78	0.49
6:T:458:PRO:O	6:T:462:LYS:HG3	2.13	0.49
6:T:461:LYS:O	6:T:465:MET:HG2	2.12	0.49
6:T:1039:TYR:CZ	6:T:1043:LEU:HD21	2.48	0.49
6:T:1832:LYS:CA	6:T:1832:LYS:CE	2.85	0.49
6:T:1864:LEU:HD11	6:T:1893:PHE:CZ	2.48	0.49
6:T:1903:GLN:HB3	6:T:1941:LEU:HD21	1.94	0.49
6:T:1992:HIS:HB2	6:T:1993:PRO:HD3	1.95	0.49
6:T:2573:LYS:O	6:T:2574:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2855:ALA:HB1	6:T:2859:TYR:HE2	1.78	0.49
6:T:3080:ASN:OD1	6:T:3081:ALA:N	2.41	0.49
1:A:152:VAL:HG22	1:A:298:VAL:HB	1.94	0.49
2:B:49:ALA:H	2:B:68:ASP:CG	2.20	0.49
3:D:32:LEU:HD23	3:D:300:ILE:HB	1.94	0.49
6:T:95:TYR:HA	6:T:98:GLU:HG3	1.94	0.49
6:T:560:MET:CB	6:T:1767:PHE:CE1	2.96	0.49
6:T:571:LEU:C	6:T:1940:TYR:HD2	2.19	0.49
6:T:730:GLU:HB3	6:T:733:SER:OG	2.13	0.49
6:T:1535:LEU:C	6:T:1535:LEU:CD2	2.86	0.49
6:T:1809:SER:HA	6:T:1812:ILE:HG12	1.95	0.49
6:T:1918:PHE:CE2	6:T:1920:ILE:HG13	2.48	0.49
6:T:1927:PHE:HA	6:T:1930:LEU:CD1	2.43	0.49
6:T:2659:GLU:HB3	6:T:2682:ARG:HD2	1.93	0.49
1:A:18:LYS:HG2	1:A:30:VAL:HG12	1.94	0.48
3:D:292:TYR:HE2	5:F:524:MET:HG2	1.78	0.48
3:D:585:ILE:HG22	3:D:587:LYS:NZ	2.28	0.48
6:T:789:ASN:HB3	6:T:828:TYR:HE1	1.77	0.48
6:T:1109:HIS:O	6:T:1113:LEU:HG	2.13	0.48
6:T:1570:LEU:C	6:T:1570:LEU:CD2	2.86	0.48
6:T:1747:PHE:HA	6:T:1750:PHE:CE2	2.48	0.48
6:T:1798:ALA:HA	6:T:1801:PHE:HD2	1.77	0.48
6:T:2100:LEU:C	6:T:2100:LEU:CD2	2.86	0.48
6:T:2172:PHE:HB2	6:T:2215:LYS:HD3	1.94	0.48
6:T:2272:VAL:N	6:T:2273:PRO:CD	2.75	0.48
6:T:2419:PRO:O	6:T:2422:VAL:HG12	2.12	0.48
6:T:2817:CYS:SG	6:T:2853:LEU:HD21	2.53	0.48
4:E:197:THR:OG1	4:E:199:GLU:OE1	2.19	0.48
6:T:24:ARG:NE	6:T:74:LYS:HB2	2.28	0.48
6:T:326:PRO:HB2	6:T:367:LEU:HD22	1.93	0.48
6:T:3169:PHE:O	6:T:3173:THR:HG23	2.12	0.48
6:T:3225:SER:HB3	6:T:3349:PHE:HE1	1.78	0.48
6:T:3270:PRO:HG2	6:T:3307:TYR:CD2	2.48	0.48
3:D:585:ILE:HD12	3:D:585:ILE:H	1.76	0.48
3:D:628:ASN:OD1	3:D:629:HIS:N	2.40	0.48
6:T:594:LEU:HD13	6:T:637:LEU:HD11	1.95	0.48
6:T:742:ARG:CZ	6:T:1544:ALA:CB	2.90	0.48
6:T:965:ASP:N	6:T:965:ASP:OD1	2.46	0.48
6:T:1762:LEU:C	6:T:1762:LEU:CD2	2.85	0.48
6:T:2711:GLN:NE2	6:T:2730:GLU:HA	2.28	0.48
6:T:3238:LYS:HG2	6:T:3407:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:312:THR:H	6:T:3629:GLN:NE2	2.12	0.48
4:E:173:PHE:HA	4:E:176:CYS:HB2	1.94	0.48
6:T:370:LEU:O	6:T:374:ARG:NH1	2.47	0.48
6:T:573:PRO:HD3	6:T:1940:TYR:CD2	2.48	0.48
6:T:851:LEU:N	6:T:852:PRO:HD3	2.28	0.48
6:T:1128:THR:OG1	6:T:1129:PHE:N	2.46	0.48
6:T:1590:SER:HB3	6:T:1593:ARG:CD	2.43	0.48
6:T:3679:HIS:O	6:T:3681:PRO:HD3	2.14	0.48
6:T:63:PRO:O	6:T:64:ILE:HD13	2.14	0.48
6:T:629:GLU:OE2	6:T:1717:GLN:CB	2.59	0.48
6:T:1039:TYR:CE1	6:T:2497:PRO:HB2	2.49	0.48
6:T:1123:ARG:HH11	6:T:1133:LEU:HD22	1.78	0.48
6:T:1703:LEU:C	6:T:1703:LEU:CD2	2.85	0.48
6:T:1800:ILE:HA	6:T:1803:LEU:CD1	2.43	0.48
6:T:1895:LYS:HD2	6:T:1895:LYS:N	2.28	0.48
6:T:2285:LEU:CD2	6:T:2311:LEU:HD11	2.44	0.48
5:F:627:LEU:HD12	5:F:628:GLU:N	2.28	0.48
6:T:247:PRO:HG2	6:T:251:PRO:HD3	1.95	0.48
6:T:462:LYS:O	6:T:466:ILE:HG13	2.13	0.48
6:T:842:LEU:HA	6:T:845:MET:HB3	1.95	0.48
6:T:2788:THR:HG22	6:T:2791:ARG:HH11	1.78	0.48
6:T:2852:PHE:O	6:T:2856:THR:HG23	2.13	0.48
6:T:3114:SER:OG	6:T:3115:GLY:N	2.46	0.48
6:T:3365:ASN:HB2	6:T:3368:PHE:CE2	2.49	0.48
1:A:169:PHE:CZ	3:D:381:VAL:HG22	2.49	0.48
2:B:175:THR:O	4:E:189:ARG:NH1	2.46	0.48
2:B:267:LYS:HD3	2:B:281:ASP:HA	1.96	0.48
3:D:594:ASP:OD1	3:D:594:ASP:N	2.45	0.48
6:T:572:LEU:N	6:T:1940:TYR:CE2	2.82	0.48
6:T:1031:SER:HB2	6:T:2493:CYS:SG	2.53	0.48
6:T:1359:PHE:HA	6:T:1362:SER:OG	2.13	0.48
6:T:2460:TRP:CG	6:T:2461:GLU:N	2.81	0.48
3:D:558:THR:HB	3:D:561:GLN:HB2	1.95	0.48
3:D:661:ASN:O	3:D:665:TYR:HB2	2.13	0.48
6:T:338:SER:O	6:T:338:SER:OG	2.31	0.48
6:T:378:GLY:O	6:T:1856:HIS:CD2	2.67	0.48
6:T:466:ILE:CA	6:T:1716:LEU:HD21	2.42	0.48
6:T:509:ASP:OD1	6:T:509:ASP:N	2.42	0.48
6:T:629:GLU:OE2	6:T:1717:GLN:N	2.46	0.48
6:T:2700:TRP:HD1	6:T:2736:CYS:SG	2.36	0.48
6:T:3177:ASP:O	6:T:3181:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:3371:ILE:HG22	6:T:3393:ILE:HG21	1.96	0.48
1:A:120:THR:HG21	1:A:370:VAL:HB	1.96	0.48
2:B:299:ASP:H	2:B:300:ILE:HD12	1.78	0.48
3:D:684:TYR:OH	6:T:2738:GLU:OE1	2.21	0.48
6:T:249:PHE:CG	6:T:289:PRO:HG3	2.49	0.48
6:T:480:ARG:CZ	6:T:1760:TYR:HB2	2.41	0.48
6:T:1300:ASN:ND2	6:T:1302:LYS:HB2	2.29	0.48
6:T:1582:ARG:HD3	6:T:1582:ARG:C	2.39	0.48
6:T:1591:PRO:HG2	6:T:1592:PHE:HD1	1.78	0.48
6:T:1974:MET:HA	6:T:1977:ASN:HB2	1.95	0.48
6:T:2118:LEU:C	6:T:2118:LEU:CD2	2.86	0.48
6:T:2244:THR:HB	6:T:2277:PRO:HB3	1.96	0.48
6:T:3151:MET:HA	6:T:3154:HIS:HD2	1.78	0.48
6:T:44:TYR:HB3	6:T:48:LEU:HD22	1.96	0.48
6:T:472:MET:HA	6:T:475:PHE:CE2	2.49	0.48
6:T:740:LEU:O	6:T:744:LEU:HD23	2.14	0.48
6:T:951:LYS:HA	6:T:2887:ARG:HE	1.79	0.48
6:T:1330:LYS:HG3	6:T:1331:GLN:N	2.29	0.48
6:T:1738:ARG:NE	6:T:1738:ARG:HA	2.29	0.48
6:T:1990:ILE:HG13	6:T:1997:PHE:CZ	2.49	0.48
6:T:2325:LEU:HD21	6:T:2328:SER:C	2.39	0.48
6:T:2898:TRP:HZ3	6:T:2949:ARG:HG3	1.79	0.48
6:T:2989:ALA:HA	6:T:3006:ILE:HD12	1.96	0.48
1:A:14:SER:HB2	1:A:158:GLY:N	2.28	0.47
1:A:349:LEU:HD12	1:A:350:THR:H	1.78	0.47
3:D:697:PHE:O	3:D:701:VAL:HG23	2.14	0.47
5:F:573:ASP:OD1	5:F:574:ARG:HD3	2.14	0.47
6:T:627:SER:H	6:T:630:GLU:CD	2.22	0.47
6:T:1190:ILE:HG23	6:T:1191:PRO:HD3	1.95	0.47
6:T:1516:VAL:CG2	6:T:1562:LEU:HD11	2.44	0.47
6:T:1879:ILE:HD12	6:T:1882:ILE:HG21	1.96	0.47
6:T:1924:THR:HA	6:T:1927:PHE:CD2	2.49	0.47
3:D:628:ASN:N	6:T:2591:TYR:HE2	2.12	0.47
5:F:520:VAL:N	5:F:523:LYS:HB3	2.29	0.47
6:T:1086:VAL:O	6:T:1090:THR:HG23	2.14	0.47
6:T:1516:VAL:HG21	6:T:1562:LEU:HD11	1.95	0.47
1:A:39:ARG:O	1:A:40:HIS:ND1	2.47	0.47
1:A:139:VAL:HG13	1:A:140:LEU:HD22	1.94	0.47
3:D:765:ARG:NE	4:E:300:MET:SD	2.74	0.47
4:E:296:THR:OG1	4:E:297:SER:N	2.48	0.47
6:T:1108:ASP:HB2	6:T:2522:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1651:TYR:HE2	6:T:1669:MET:HB3	1.78	0.47
6:T:1741:ASN:HB3	6:T:1742:PRO:HD3	1.96	0.47
6:T:1872:ILE:HD12	6:T:1912:PHE:CD2	2.49	0.47
6:T:1919:PRO:HD2	6:T:1923:VAL:HG23	1.96	0.47
6:T:3464:PHE:HB3	6:T:3575:ASP:HA	1.95	0.47
6:T:3731:ARG:H	6:T:3731:ARG:HD2	1.80	0.47
4:E:298:GLN:OE1	4:E:299:GLY:N	2.47	0.47
6:T:428:ALA:HB3	6:T:431:VAL:HG12	1.96	0.47
6:T:1040:THR:OG1	6:T:1041:GLU:N	2.47	0.47
6:T:1290:THR:HG22	6:T:1329:SER:OG	2.15	0.47
6:T:1547:MET:N	6:T:1548:PRO:CD	2.78	0.47
6:T:1644:LEU:HA	6:T:1647:PHE:CD2	2.50	0.47
6:T:1747:PHE:HA	6:T:1750:PHE:CZ	2.50	0.47
6:T:2122:ASN:N	6:T:2122:ASN:ND2	2.60	0.47
6:T:2177:LYS:NZ	6:T:2179:TRP:HB3	2.30	0.47
6:T:3371:ILE:HG13	6:T:3371:ILE:O	2.15	0.47
6:T:3493:LEU:HD11	6:T:3506:MET:HE1	1.95	0.47
1:A:36:GLY:HA3	1:A:53:TYR:HB2	1.96	0.47
5:F:580:HIS:CG	5:F:581:LEU:H	2.32	0.47
6:T:242:THR:HB	6:T:328:LEU:HD21	1.97	0.47
6:T:605:ASN:HD22	6:T:620:ALA:C	2.22	0.47
6:T:678:ASP:OD1	6:T:679:ALA:N	2.48	0.47
6:T:1046:ALA:O	6:T:1049:SER:OG	2.22	0.47
6:T:1240:GLY:O	6:T:1244:VAL:HG23	2.14	0.47
6:T:1556:ILE:HD12	6:T:1573:LEU:HD21	1.95	0.47
6:T:1744:LEU:HA	6:T:1747:PHE:CD2	2.50	0.47
6:T:1744:LEU:HD13	6:T:1747:PHE:CE2	2.50	0.47
6:T:1985:LEU:HA	6:T:1988:PHE:CZ	2.49	0.47
6:T:2003:PHE:HA	6:T:2006:ASN:ND2	2.29	0.47
6:T:2158:LEU:H	6:T:2158:LEU:CD1	2.28	0.47
6:T:2557:HIS:ND1	6:T:2605:MET:HG2	2.29	0.47
6:T:3464:PHE:HB2	6:T:3574:VAL:O	2.14	0.47
1:A:30:VAL:HG11	1:A:337:TYR:CE1	2.50	0.47
1:A:39:ARG:NE	1:A:63:GLY:O	2.48	0.47
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.49	0.47
1:A:253:GLU:H	1:A:253:GLU:CD	2.21	0.47
3:D:623:TYR:HD1	3:D:626:ARG:HH21	1.63	0.47
6:T:638:PHE:O	6:T:642:ILE:HG12	2.14	0.47
6:T:1068:ASN:ND2	6:T:1071:ASP:OD2	2.46	0.47
6:T:1219:LEU:O	6:T:1223:VAL:HG12	2.14	0.47
6:T:1289:LEU:O	6:T:1293:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1658:ASN:HD21	6:T:1665:PHE:HZ	1.61	0.47
6:T:2679:TRP:CZ3	6:T:2728:LEU:HD22	2.50	0.47
6:T:2959:MET:O	6:T:2959:MET:HG2	2.15	0.47
6:T:3119:ASN:O	6:T:3123:SER:OG	2.17	0.47
2:B:152:ARG:NH2	2:B:440:LEU:HD11	2.30	0.47
3:D:346:LYS:HE2	5:F:536:PHE:HD2	1.79	0.47
4:E:271:THR:O	4:E:275:ARG:HG2	2.13	0.47
6:T:28:LEU:HG	6:T:78:SER:HB3	1.97	0.47
6:T:159:PHE:HE1	6:T:298:GLN:HE22	1.62	0.47
6:T:638:PHE:HB2	6:T:690:PHE:CZ	2.49	0.47
6:T:687:ALA:O	6:T:691:MET:HG2	2.15	0.47
6:T:1907:LEU:C	6:T:1907:LEU:CD2	2.85	0.47
6:T:1998:ASN:ND2	6:T:2041:LYS:HG2	2.29	0.47
6:T:2034:LEU:C	6:T:2034:LEU:CD2	2.86	0.47
6:T:2168:LEU:HD11	6:T:2211:GLN:CG	2.45	0.47
6:T:2182:GLU:CD	6:T:2182:GLU:N	2.73	0.47
6:T:2238:MET:SD	6:T:2239:LEU:N	2.88	0.47
6:T:2359:TRP:HA	6:T:2362:ASN:CG	2.40	0.47
6:T:2374:ALA:O	6:T:2378:LYS:HG2	2.14	0.47
6:T:2379:MET:HE3	6:T:2382:PHE:CE2	2.49	0.47
6:T:2961:ASP:OD1	6:T:2961:ASP:N	2.47	0.47
6:T:3110:ILE:HG22	6:T:3112:ASP:H	1.78	0.47
6:T:3418:ARG:NH1	6:T:3669:ASP:HB3	2.30	0.47
6:T:3564:ILE:HA	6:T:3588:PRO:HA	1.95	0.47
6:T:3731:ARG:O	6:T:3735:ARG:HG3	2.14	0.47
3:D:590:VAL:HA	5:F:570:PHE:CE2	2.50	0.47
4:E:169:ILE:O	4:E:173:PHE:CB	2.63	0.47
4:E:194:ASN:OD1	4:E:195:SER:N	2.48	0.47
6:T:1794:LYS:HD3	6:T:1794:LYS:N	2.27	0.47
6:T:2008:ILE:CG1	6:T:2031:LEU:HD21	2.44	0.47
6:T:2129:SER:HB3	6:T:2173:LYS:NZ	2.30	0.47
6:T:2304:ALA:HA	6:T:2307:THR:HG22	1.96	0.47
1:A:242:LEU:HB2	1:A:246:GLN:HB3	1.96	0.47
3:D:533:GLU:HG2	3:D:533:GLU:O	2.15	0.47
6:T:328:LEU:O	6:T:332:LEU:HG	2.15	0.47
6:T:2235:PHE:HA	6:T:2238:MET:HG3	1.97	0.47
1:A:190:MET:HG3	1:A:200:PHE:HB2	1.96	0.47
2:B:183:ASN:ND2	2:B:185:ILE:HB	2.31	0.47
6:T:418:TYR:HA	6:T:421:TYR:CD2	2.50	0.47
6:T:744:LEU:HD12	6:T:766:PHE:CE2	2.50	0.47
6:T:935:GLN:C	6:T:937:PHE:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1751:SER:HA	6:T:1799:ARG:NE	2.30	0.47
6:T:1864:LEU:HD13	6:T:1889:PHE:CZ	2.50	0.47
6:T:2594:ARG:HH12	6:T:2603:ILE:HD12	1.80	0.47
6:T:3420:PHE:HE1	6:T:3446:PRO:HD2	1.80	0.47
1:A:349:LEU:HD21	3:D:390:ALA:HB1	1.97	0.46
3:D:51:GLN:NE2	3:D:54:GLU:OE2	2.42	0.46
3:D:323:ARG:NH1	5:F:561:PRO:HD3	2.30	0.46
6:T:76:ARG:O	6:T:80:LEU:HG	2.16	0.46
6:T:857:LEU:O	6:T:861:LEU:HG	2.15	0.46
6:T:1053:GLU:OE1	6:T:1053:GLU:N	2.48	0.46
6:T:1876:PRO:HA	6:T:1883:LYS:HE2	1.96	0.46
6:T:2236:ILE:HD12	6:T:2263:LEU:HD22	1.97	0.46
6:T:2316:TYR:CE2	6:T:2348:PHE:CD2	3.03	0.46
6:T:2348:PHE:O	6:T:2352:ILE:HG23	2.15	0.46
6:T:2545:LEU:HG	6:T:2549:PHE:CE2	2.49	0.46
6:T:2610:ILE:HG21	6:T:2618:LEU:HD23	1.96	0.46
6:T:3136:PHE:O	6:T:3140:LEU:HG	2.15	0.46
6:T:3322:GLU:OE2	6:T:3382:ARG:NH2	2.48	0.46
6:T:382:THR:HG21	6:T:1901:ILE:HD11	1.98	0.46
6:T:1796:LEU:HD12	6:T:1799:ARG:HD3	1.98	0.46
6:T:2422:VAL:HA	6:T:2425:ARG:HG2	1.98	0.46
6:T:3332:GLU:HB2	6:T:3378:VAL:HG13	1.97	0.46
1:A:94:LEU:HB3	1:A:96:VAL:HG12	1.98	0.46
3:D:53:LEU:HA	3:D:53:LEU:HD23	1.62	0.46
3:D:588:SER:OG	3:D:589:VAL:N	2.48	0.46
3:D:618:ARG:C	3:D:619:ARG:HD2	2.39	0.46
4:E:186:ILE:O	4:E:190:TYR:HB3	2.15	0.46
4:E:206:TYR:HA	4:E:209:CYS:SG	2.56	0.46
6:T:381:PHE:HD2	6:T:1859:LEU:CD2	2.21	0.46
6:T:382:THR:H	6:T:1858:ASP:CG	2.23	0.46
6:T:1860:PHE:HD2	6:T:1861:ARG:HD2	1.80	0.46
6:T:2101:ILE:HD12	6:T:2166:ASP:HB3	1.96	0.46
6:T:3081:ALA:HB1	6:T:3085:TYR:HE1	1.81	0.46
1:A:216:LEU:HB3	1:A:254:ARG:HE	1.78	0.46
1:A:342:GLY:HA2	1:A:345:ILE:HD12	1.96	0.46
2:B:108:ALA:O	2:B:137:CYS:HA	2.15	0.46
2:B:389:VAL:O	2:B:392:SER:OG	2.29	0.46
6:T:471:TYR:HE2	6:T:593:PHE:HD2	1.63	0.46
6:T:481:GLN:O	6:T:485:ILE:HG13	2.16	0.46
6:T:1442:ALA:O	6:T:1446:LYS:HG3	2.15	0.46
6:T:1799:ARG:N	6:T:1799:ARG:CD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2007:ILE:CD1	6:T:2031:LEU:HD13	2.45	0.46
6:T:2182:GLU:HG2	6:T:2183:ASN:ND2	2.30	0.46
6:T:3423:TYR:HB2	6:T:3445:LEU:HD13	1.97	0.46
6:T:3499:ASP:OD1	6:T:3499:ASP:N	2.48	0.46
1:A:338:SER:HA	1:A:341:ILE:HD12	1.96	0.46
2:B:13:GLU:OE2	5:F:644:ARG:NH1	2.38	0.46
3:D:587:LYS:HD2	4:E:244:LEU:HD21	1.97	0.46
3:D:650:TRP:CE3	3:D:699:ARG:HG2	2.50	0.46
6:T:384:HIS:CD2	6:T:387:LEU:HD12	2.51	0.46
6:T:438:LEU:O	6:T:442:LEU:HG	2.16	0.46
6:T:517:PHE:O	6:T:521:VAL:HG22	2.15	0.46
6:T:719:LEU:HA	6:T:722:VAL:HG23	1.98	0.46
6:T:723:ALA:O	6:T:727:LEU:HD22	2.16	0.46
6:T:742:ARG:NH2	6:T:1544:ALA:HB3	2.30	0.46
6:T:963:PRO:HD2	6:T:3543:LEU:HD21	1.97	0.46
6:T:1518:ILE:HA	6:T:1521:LYS:CE	2.46	0.46
6:T:2282:PHE:HD2	6:T:2315:LEU:HG	1.81	0.46
1:A:312:ARG:O	1:A:316:GLU:HG2	2.16	0.46
2:B:45:GLY:HA3	2:B:69:TYR:OH	2.16	0.46
3:D:767:CYS:SG	6:T:2704:GLN:NE2	2.89	0.46
6:T:37:LEU:HD23	6:T:37:LEU:H	1.80	0.46
6:T:345:LYS:O	6:T:349:HIS:ND1	2.30	0.46
6:T:1268:LEU:O	6:T:1272:PHE:HB2	2.15	0.46
6:T:3021:GLU:OE1	6:T:3021:GLU:N	2.48	0.46
6:T:3733:LEU:O	6:T:3736:THR:HG22	2.15	0.46
1:A:61:LYS:HG2	1:A:64:ILE:HD11	1.98	0.46
1:A:213:LYS:HD3	1:A:306:PHE:CZ	2.51	0.46
6:T:685:TYR:O	6:T:689:MET:HG3	2.15	0.46
6:T:1188:SER:OG	6:T:1189:PHE:N	2.48	0.46
6:T:1510:LEU:HA	6:T:1513:TYR:CE1	2.50	0.46
6:T:1597:ALA:HB2	6:T:1627:ILE:HG23	1.97	0.46
6:T:1966:TRP:CD1	6:T:1966:TRP:H	2.31	0.46
6:T:2229:GLU:HA	6:T:2229:GLU:OE2	2.15	0.46
6:T:2332:PHE:O	6:T:2335:THR:OG1	2.23	0.46
6:T:3339:PRO:O	6:T:3343:ASN:ND2	2.48	0.46
6:T:3416:GLU:OE1	6:T:3586:MET:N	2.49	0.46
2:B:83:TRP:CH2	2:B:124:SER:HB3	2.51	0.46
5:F:585:LEU:C	5:F:586:LYS:HD3	2.41	0.46
6:T:69:HIS:HA	6:T:73:GLN:HG3	1.97	0.46
6:T:293:ASP:OD1	6:T:294:PHE:N	2.49	0.46
6:T:683:MET:HB3	6:T:722:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:700:GLU:OE1	6:T:1587:GLN:N	2.42	0.46
6:T:1110:PHE:CZ	6:T:1144:LEU:HD11	2.50	0.46
6:T:1320:ILE:HG13	6:T:1325:LEU:HD21	1.97	0.46
6:T:1640:PHE:HB3	6:T:1672:LEU:HD21	1.96	0.46
6:T:2485:GLU:HG2	6:T:2486:LEU:N	2.28	0.46
6:T:3416:GLU:HG3	6:T:3420:PHE:HE2	1.80	0.46
6:T:3721:LEU:HA	6:T:3724:ILE:HG22	1.97	0.46
1:A:120:THR:HG22	1:A:132:PHE:HE2	1.81	0.46
3:D:534:GLU:OE2	5:F:641:ARG:NH2	2.30	0.46
5:F:586:LYS:HE2	5:F:586:LYS:HB2	1.78	0.46
6:T:148:TYR:CG	6:T:241:LEU:HD11	2.51	0.46
6:T:480:ARG:HH11	6:T:1760:TYR:HD1	0.71	0.46
6:T:685:TYR:C	6:T:689:MET:HE3	2.41	0.46
6:T:1185:LEU:HD21	6:T:1229:PHE:HB3	1.98	0.46
6:T:1453:PRO:HA	6:T:1456:ILE:HG12	1.98	0.46
6:T:1473:LEU:C	6:T:1473:LEU:CD2	2.85	0.46
6:T:1629:GLN:HA	6:T:1675:THR:HG23	1.98	0.46
6:T:1877:GLU:CD	6:T:1877:GLU:N	2.73	0.46
6:T:1910:SER:HA	6:T:1913:ILE:CD1	2.45	0.46
6:T:2096:CYS:SG	6:T:2097:THR:N	2.88	0.46
6:T:2704:GLN:HG3	6:T:2733:TRP:NE1	2.29	0.46
6:T:3419:MET:HE3	6:T:3588:PRO:HG2	1.97	0.46
2:B:462:LEU:HD11	2:B:465:PHE:HB2	1.98	0.46
3:D:683:SER:HB2	6:T:2731:ASP:HB3	1.99	0.46
6:T:382:THR:N	6:T:1858:ASP:OD2	2.44	0.46
6:T:848:THR:OG1	6:T:849:ALA:N	2.49	0.46
6:T:1311:LEU:HD13	6:T:1314:ILE:HD11	1.98	0.46
6:T:1358:THR:HA	6:T:1418:LEU:HD13	1.98	0.46
6:T:1526:LEU:CD2	6:T:1552:ILE:HG23	2.46	0.46
6:T:1645:ASP:HA	6:T:1648:TYR:HD2	1.79	0.46
6:T:1750:PHE:HD1	6:T:1750:PHE:C	2.24	0.46
6:T:2538:SER:O	6:T:2542:ILE:HG12	2.16	0.46
6:T:2665:LEU:HD12	6:T:2665:LEU:HA	1.80	0.46
6:T:3331:LYS:HE2	6:T:3377:THR:HB	1.97	0.46
2:B:240:GLN:OE1	7:B:501:ATP:O2'	2.29	0.45
2:B:462:LEU:HD12	2:B:464:THR:H	1.80	0.45
3:D:258:TYR:HB2	5:F:627:LEU:HD21	1.98	0.45
6:T:93:GLN:O	6:T:97:MET:HG2	2.16	0.45
6:T:444:GLU:O	6:T:447:LEU:HG	2.16	0.45
6:T:1438:ILE:HA	6:T:1473:LEU:HD11	1.98	0.45
6:T:1939:ARG:CZ	6:T:1939:ARG:CB	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2011:MET:HA	6:T:2014:ILE:HG12	1.97	0.45
6:T:2174:ASN:HB3	6:T:2175:LYS:NZ	2.31	0.45
6:T:2393:LEU:O	6:T:2397:ILE:HG23	2.16	0.45
6:T:2651:ASN:O	6:T:2654:ILE:HG22	2.15	0.45
6:T:3411:ARG:NH1	6:T:3412:HIS:HB3	2.32	0.45
1:A:173:HIS:CD2	2:B:446:ILE:HG21	2.51	0.45
4:E:269:LYS:C	4:E:270:ARG:HE	2.22	0.45
6:T:73:GLN:HE22	6:T:116:ILE:HD11	1.80	0.45
6:T:952:LEU:O	6:T:956:ASN:N	2.49	0.45
6:T:1223:VAL:HG13	6:T:1230:LEU:HD21	1.98	0.45
6:T:1441:LEU:CB	6:T:1473:LEU:HD11	2.26	0.45
6:T:2180:ILE:CD1	6:T:2183:ASN:HB2	2.46	0.45
6:T:2454:VAL:HG21	6:T:2472:ALA:HA	1.98	0.45
2:B:178:LYS:H	4:E:188:ASP:CG	2.22	0.45
4:E:289:GLN:HE22	4:E:292:THR:HA	1.82	0.45
6:T:1267:LEU:O	6:T:1271:THR:HG22	2.17	0.45
6:T:1412:ARG:O	6:T:1416:ILE:HG13	2.16	0.45
6:T:1564:PRO:HA	6:T:1603:PHE:HE1	1.81	0.45
6:T:1848:ILE:CB	6:T:1852:ASP:HB2	2.46	0.45
6:T:3687:GLN:O	6:T:3691:MET:HG3	2.15	0.45
2:B:60:GLN:NE2	2:B:60:GLN:O	2.50	0.45
3:D:59:ASN:ND2	3:D:63:LYS:HG3	2.32	0.45
6:T:123:THR:O	6:T:127:LYS:HG3	2.16	0.45
6:T:393:SER:HA	6:T:434:MET:HE1	1.98	0.45
6:T:462:LYS:HZ3	6:T:1715:HIS:HE2	1.62	0.45
6:T:515:GLU:OE2	6:T:519:ARG:NH2	2.50	0.45
6:T:570:LEU:HD21	6:T:1940:TYR:OH	2.17	0.45
6:T:853:HIS:HB3	6:T:856:GLU:CG	2.45	0.45
6:T:1060:ASN:HD22	6:T:1134:LYS:NZ	2.15	0.45
6:T:1172:TYR:HD2	6:T:1190:ILE:HD12	1.81	0.45
6:T:1299:ALA:HA	6:T:1304:ARG:NH1	2.31	0.45
6:T:1449:LEU:CD2	6:T:1484:PRO:CB	2.94	0.45
6:T:1546:GLN:CG	6:T:1548:PRO:HD2	2.46	0.45
6:T:1677:VAL:HG21	6:T:1728:LEU:HD11	1.98	0.45
6:T:2285:LEU:HD13	6:T:2312:GLU:HG3	1.99	0.45
6:T:2366:PHE:O	6:T:2368:THR:N	2.50	0.45
2:B:160:ILE:HG22	2:B:414:THR:OG1	2.16	0.45
2:B:431:ILE:HG23	2:B:432:LEU:H	1.81	0.45
2:B:473:LYS:H	2:B:473:LYS:HD2	1.81	0.45
3:D:302:LEU:HD21	4:E:279:LEU:HB3	1.98	0.45
6:T:593:PHE:O	6:T:596:THR:OG1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1330:LYS:HG3	6:T:1331:GLN:H	1.82	0.45
6:T:1618:ARG:HA	6:T:1621:VAL:HG22	1.99	0.45
6:T:2461:GLU:HG3	6:T:2592:HIS:CB	2.47	0.45
6:T:2542:ILE:O	6:T:2546:ILE:HG12	2.16	0.45
6:T:2620:PRO:C	6:T:2622:LEU:H	2.24	0.45
6:T:2663:LEU:HD13	6:T:2679:TRP:NE1	2.31	0.45
6:T:3620:VAL:HG23	6:T:3727:ALA:HA	1.98	0.45
6:T:3635:SER:OG	6:T:3636:ALA:N	2.49	0.45
1:A:96:VAL:HG22	1:A:101:HIS:HE2	1.81	0.45
1:A:215:LYS:HB3	1:A:216:LEU:HD12	1.99	0.45
3:D:321:GLU:O	3:D:324:ILE:HG22	2.16	0.45
6:T:45:HIS:HB2	6:T:88:MET:HE1	1.99	0.45
6:T:766:PHE:O	6:T:769:SER:OG	2.27	0.45
6:T:849:ALA:HB3	6:T:854:GLU:CB	2.47	0.45
6:T:1864:LEU:HD13	6:T:1889:PHE:HZ	1.82	0.45
6:T:1939:ARG:HE	6:T:1985:LEU:HD22	1.81	0.45
6:T:2369:VAL:HG12	6:T:2372:LYS:HD3	1.99	0.45
6:T:2597:SER:OG	6:T:2598:SER:N	2.49	0.45
6:T:2986:ARG:HH12	6:T:2990:LYS:HZ1	1.64	0.45
6:T:3160:ALA:HA	6:T:3167:LEU:HD21	1.97	0.45
1:A:357:ILE:HD11	1:A:373:LYS:HB2	1.98	0.45
2:B:472:LYS:O	2:B:476:GLU:HG2	2.16	0.45
6:T:76:ARG:HA	6:T:79:MET:SD	2.57	0.45
6:T:460:ALA:O	6:T:464:LEU:HG	2.17	0.45
6:T:466:ILE:CG1	6:T:1716:LEU:HD11	2.46	0.45
6:T:850:ARG:NH2	6:T:1007:TYR:HB2	2.31	0.45
6:T:1715:HIS:ND1	6:T:1717:GLN:HG2	2.31	0.45
6:T:2292:ILE:C	6:T:2295:PRO:HD2	2.42	0.45
6:T:2325:LEU:CD2	6:T:2329:ARG:CB	2.95	0.45
6:T:2353:VAL:HA	6:T:2356:SER:OG	2.16	0.45
6:T:2506:GLU:OE1	6:T:2507:ASN:ND2	2.50	0.45
6:T:2681:ARG:HH11	6:T:3634:ASP:HB2	1.81	0.45
6:T:3087:GLN:HG2	6:T:3124:PHE:CE1	2.50	0.45
6:T:3288:LEU:O	6:T:3292:ILE:HG22	2.16	0.45
2:B:23:SER:OG	7:B:501:ATP:O3B	2.30	0.45
2:B:172:ASP:OD2	4:E:182:ARG:NH1	2.50	0.45
4:E:213:PHE:O	4:E:217:ASP:N	2.50	0.45
6:T:472:MET:HE3	6:T:472:MET:HB3	1.85	0.45
6:T:949:LEU:HD23	6:T:949:LEU:HA	1.78	0.45
6:T:1251:GLU:H	6:T:1251:GLU:CD	2.17	0.45
6:T:1491:ASP:HA	6:T:1525:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1800:ILE:HA	6:T:1803:LEU:HD12	1.98	0.45
6:T:2179:TRP:HA	6:T:2181:MET:CE	2.46	0.45
6:T:2418:GLN:HB3	6:T:2419:PRO:HD3	1.99	0.45
6:T:2554:LYS:HE3	6:T:2558:ARG:HH21	1.82	0.45
1:A:66:THR:HG1	1:A:68:ARG:HH22	1.61	0.45
1:A:287:VAL:HA	1:A:290:ARG:NE	2.32	0.45
1:A:354:GLN:HG3	1:A:355:MET:SD	2.56	0.45
3:D:23:ARG:HH21	3:D:27:PRO:HG3	1.82	0.45
6:T:90:GLN:HG2	6:T:91:THR:HG23	1.97	0.45
6:T:409:SER:O	6:T:412:GLU:HG3	2.16	0.45
6:T:629:GLU:O	6:T:633:VAL:HG13	2.16	0.45
6:T:641:CYS:O	6:T:645:LEU:HG	2.17	0.45
6:T:1266:ASP:O	6:T:1269:SER:OG	2.30	0.45
6:T:1564:PRO:HD3	6:T:1602:ARG:CZ	2.47	0.45
6:T:1676:MET:HE2	6:T:1676:MET:HB3	1.84	0.45
6:T:1952:VAL:HA	6:T:1955:GLU:HG2	1.99	0.45
6:T:2677:GLY:HA3	6:T:3639:GLY:HA3	1.98	0.45
6:T:3295:LYS:HG3	6:T:3317:TRP:HZ2	1.82	0.45
1:A:177:ARG:NH2	2:B:96:ASN:O	2.40	0.45
2:B:402:ALA:HA	2:B:435:LEU:HD22	1.99	0.45
3:D:628:ASN:O	6:T:2591:TYR:OH	2.35	0.45
3:D:669:TRP:CZ2	3:D:697:PHE:HD1	2.34	0.45
6:T:422:LEU:O	6:T:432:GLN:NE2	2.51	0.45
6:T:705:GLU:O	6:T:709:VAL:HG23	2.17	0.45
6:T:738:GLY:O	6:T:742:ARG:HG3	2.16	0.45
6:T:854:GLU:HG2	6:T:855:ARG:N	2.32	0.45
6:T:1133:LEU:HD23	6:T:1133:LEU:HA	1.80	0.45
6:T:1258:ASP:OD1	6:T:1259:SER:N	2.51	0.45
6:T:1605:ASN:N	6:T:1606:PRO:CD	2.80	0.45
6:T:1768:HIS:C	6:T:1768:HIS:CD2	2.94	0.45
6:T:1918:PHE:CD1	6:T:1923:VAL:HG21	2.51	0.45
6:T:1939:ARG:HB3	6:T:1939:ARG:NH1	2.31	0.45
6:T:2094:GLU:C	6:T:2094:GLU:CD	2.85	0.45
6:T:2412:ILE:O	6:T:2415:ARG:HG2	2.17	0.45
6:T:2518:GLU:OE1	6:T:2521:ASN:ND2	2.48	0.45
2:B:249:ILE:HD12	2:B:420:LEU:HA	1.98	0.44
2:B:434:SER:HA	4:E:251:ILE:HD12	1.99	0.44
4:E:82:GLU:OE1	4:E:82:GLU:N	2.50	0.44
6:T:249:PHE:HB3	6:T:288:ARG:NE	2.32	0.44
6:T:778:ASN:OD1	6:T:778:ASN:N	2.50	0.44
6:T:1180:GLY:HA3	6:T:1183:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1508:GLU:HB2	6:T:1561:LEU:HD12	1.99	0.44
6:T:1535:LEU:HD23	6:T:1535:LEU:O	2.16	0.44
6:T:1580:LEU:HD11	6:T:1592:PHE:CZ	2.52	0.44
6:T:2122:ASN:N	6:T:2122:ASN:HD22	2.14	0.44
6:T:2179:TRP:O	6:T:2179:TRP:CE3	2.70	0.44
6:T:2345:ASP:H	6:T:2348:PHE:HE1	1.65	0.44
6:T:3222:LEU:HD12	6:T:3222:LEU:HA	1.81	0.44
1:A:312:ARG:NE	1:A:316:GLU:OE2	2.50	0.44
4:E:194:ASN:ND2	4:E:196:ARG:HD3	2.32	0.44
6:T:339:GLU:CB	6:T:1897:GLU:HB3	2.47	0.44
6:T:345:LYS:C	6:T:349:HIS:HD1	2.18	0.44
6:T:386:THR:O	6:T:389:PRO:HD2	2.18	0.44
6:T:1018:TYR:O	6:T:1022:THR:HG23	2.17	0.44
6:T:1186:SER:OG	6:T:1187:HIS:N	2.51	0.44
6:T:1440:ILE:HA	6:T:1443:VAL:HG12	1.98	0.44
6:T:1804:LYS:HD3	6:T:1863:GLU:HG2	1.99	0.44
6:T:2412:ILE:HG23	6:T:2415:ARG:H	1.83	0.44
6:T:2542:ILE:HG13	6:T:2543:ASP:N	2.32	0.44
6:T:2596:ILE:HG13	6:T:2602:VAL:HG11	1.98	0.44
6:T:2909:PHE:O	6:T:2912:ILE:HG22	2.18	0.44
1:A:217:CYS:HA	1:A:254:ARG:HB3	1.99	0.44
3:D:605:LEU:HD21	5:F:614:ILE:HG23	2.00	0.44
3:D:665:TYR:HE2	3:D:675:HIS:CE1	2.35	0.44
6:T:932:LEU:HG	6:T:2825:LEU:HD11	1.98	0.44
6:T:1532:VAL:HG22	6:T:1583:LYS:NZ	2.32	0.44
6:T:1532:VAL:HG22	6:T:1583:LYS:CE	2.47	0.44
6:T:1748:ILE:HD11	6:T:1789:PHE:CZ	2.53	0.44
6:T:1856:HIS:CG	6:T:1856:HIS:O	2.70	0.44
6:T:1924:THR:HA	6:T:1927:PHE:CE2	2.52	0.44
6:T:2092:LEU:H	6:T:2092:LEU:HG	1.61	0.44
6:T:2230:SER:N	6:T:2231:PRO:CD	2.81	0.44
6:T:2303:GLU:N	6:T:2303:GLU:CD	2.73	0.44
6:T:2620:PRO:O	6:T:2622:LEU:N	2.50	0.44
6:T:2663:LEU:HD23	6:T:2663:LEU:HA	1.71	0.44
6:T:3251:VAL:HA	6:T:3254:ILE:HG22	1.99	0.44
6:T:3353:GLU:OE2	6:T:3358:TYR:HE2	2.00	0.44
6:T:3565:ASN:OD1	6:T:3566:ASN:N	2.45	0.44
6:T:3710:ASN:OD1	6:T:3711:SER:N	2.48	0.44
3:D:58:GLU:HG3	3:D:59:ASN:N	2.32	0.44
6:T:357:THR:O	6:T:361:LYS:HG3	2.18	0.44
6:T:474:ARG:NH2	6:T:477:THR:OG1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:518:MET:SD	6:T:2317:ILE:HG21	2.57	0.44
6:T:563:ILE:HG23	6:T:564:LYS:H	1.83	0.44
6:T:611:TYR:CE1	6:T:1585:ARG:HB3	2.52	0.44
6:T:1041:GLU:O	6:T:1045:THR:HG23	2.17	0.44
6:T:1286:GLU:OE2	6:T:1328:HIS:NE2	2.51	0.44
6:T:1641:GLU:CG	6:T:1676:MET:HE2	2.48	0.44
6:T:2124:LEU:C	6:T:2124:LEU:CD2	2.86	0.44
6:T:2573:LYS:C	6:T:2575:GLU:H	2.24	0.44
6:T:3253:LEU:HD12	6:T:3314:LEU:HB3	1.98	0.44
1:A:305:MET:HA	1:A:335:ARG:NH1	2.32	0.44
2:B:18:VAL:HG21	2:B:457:SER:HA	1.99	0.44
2:B:245:THR:HA	3:D:75:ARG:NH2	2.33	0.44
2:B:406:HIS:O	2:B:438:ARG:HG2	2.17	0.44
3:D:352:TRP:N	3:D:352:TRP:CD1	2.85	0.44
3:D:599:LYS:C	3:D:600:LEU:HD22	2.43	0.44
6:T:730:GLU:HG2	6:T:732:THR:N	2.24	0.44
6:T:806:LEU:HD12	6:T:806:LEU:H	1.82	0.44
6:T:1066:THR:N	6:T:3476:LYS:HZ2	2.15	0.44
6:T:1493:GLN:HE21	6:T:1493:GLN:CA	2.12	0.44
6:T:1539:PHE:CD2	6:T:1539:PHE:O	2.70	0.44
6:T:1685:LEU:HD12	6:T:1689:GLY:H	1.83	0.44
6:T:2175:LYS:HD3	6:T:2175:LYS:H	1.82	0.44
6:T:3075:ILE:HG23	6:T:3077:PHE:H	1.83	0.44
6:T:3134:ILE:HG12	6:T:3166:ALA:HB1	2.00	0.44
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.83	0.44
2:B:74:ILE:O	2:B:81:ILE:HG12	2.17	0.44
3:D:762:GLU:N	3:D:762:GLU:OE1	2.50	0.44
5:F:540:ASP:CG	5:F:545:PRO:HD3	2.42	0.44
6:T:724:GLN:O	6:T:728:THR:HG23	2.18	0.44
6:T:1041:GLU:HB3	6:T:2513:GLU:HB2	1.99	0.44
6:T:1798:ALA:HA	6:T:1801:PHE:CD2	2.52	0.44
6:T:1815:VAL:HG21	6:T:1870:ILE:CD1	2.47	0.44
6:T:1849:LEU:HD13	6:T:1896:LEU:HD23	2.00	0.44
6:T:1876:PRO:HA	6:T:1883:LYS:NZ	2.33	0.44
6:T:1903:GLN:HB3	6:T:1941:LEU:CD2	2.48	0.44
6:T:2328:SER:C	6:T:2331:PRO:HD2	2.43	0.44
6:T:3583:THR:HG22	6:T:3584:LEU:H	1.83	0.44
1:A:191:LYS:O	1:A:195:GLU:HG2	2.17	0.44
3:D:537:LYS:HE3	3:D:537:LYS:HB2	1.67	0.44
3:D:558:THR:O	3:D:560:ILE:HD12	2.18	0.44
3:D:615:LEU:H	6:T:2456:ARG:NH1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:247:SER:OG	4:E:248:ALA:N	2.51	0.44
4:E:269:LYS:HB3	5:F:624:GLN:HE22	1.83	0.44
5:F:573:ASP:CG	5:F:574:ARG:N	2.76	0.44
6:T:562:ASP:HB3	6:T:566:TYR:HD2	1.81	0.44
6:T:1838:HIS:CE1	6:T:1882:ILE:HD12	2.52	0.44
6:T:2036:LEU:CD2	6:T:2123:ILE:HG23	2.48	0.44
6:T:2282:PHE:HA	6:T:2285:LEU:HD12	1.99	0.44
6:T:2285:LEU:HD13	6:T:2312:GLU:CG	2.48	0.44
6:T:2432:ARG:NH1	6:T:2547:GLU:OE2	2.51	0.44
6:T:2434:ARG:O	6:T:2438:ILE:HG12	2.18	0.44
6:T:2509:GLU:N	6:T:2509:GLU:OE1	2.50	0.44
6:T:2876:GLU:OE1	6:T:2876:GLU:N	2.33	0.44
6:T:3026:LYS:O	6:T:3030:LEU:HG	2.17	0.44
1:A:6:ALA:O	1:A:101:HIS:HB3	2.17	0.44
1:A:110:MET:HB3	2:B:37:GLN:HE21	1.83	0.44
1:A:272:ALA:H	2:B:60:GLN:HE21	1.66	0.44
2:B:80:VAL:HB	2:B:120:ASN:HD21	1.83	0.44
3:D:36:ARG:HE	3:D:322:ALA:HB1	1.83	0.44
3:D:60:LYS:HD2	3:D:60:LYS:HA	1.68	0.44
3:D:81:ASP:N	3:D:81:ASP:OD1	2.51	0.44
3:D:312:THR:OG1	6:T:3626:PRO:HG3	2.18	0.44
3:D:359:GLN:O	3:D:363:LEU:HG	2.18	0.44
4:E:294:TYR:HB2	4:E:302:GLN:HG2	1.99	0.44
6:T:125:LEU:HD11	6:T:140:PHE:CZ	2.53	0.44
6:T:344:ARG:O	6:T:348:LEU:HG	2.18	0.44
6:T:1568:MET:HE3	6:T:1568:MET:O	2.17	0.44
6:T:2090:LEU:HA	6:T:2093:ARG:CD	2.47	0.44
6:T:2330:ARG:NH2	6:T:2371:GLU:OE2	2.50	0.44
6:T:2372:LYS:O	6:T:2375:ILE:HG12	2.18	0.44
6:T:2402:PHE:CZ	6:T:2416:MET:HB3	2.53	0.44
6:T:3230:VAL:HG23	6:T:3451:LEU:HD22	2.00	0.44
6:T:3426:PHE:HD1	6:T:3426:PHE:HA	1.71	0.44
1:A:10:ILE:HD11	1:A:90:PHE:CE1	2.52	0.44
6:T:712:ARG:HD3	6:T:712:ARG:HA	1.72	0.44
6:T:1345:LEU:O	6:T:1350:GLN:HG3	2.18	0.44
6:T:1879:ILE:HB	6:T:1882:ILE:CG1	2.47	0.44
6:T:1904:SER:N	6:T:1941:LEU:HD21	2.33	0.44
6:T:1918:PHE:CD2	6:T:1918:PHE:O	2.71	0.44
6:T:2490:ASN:OD1	6:T:2490:ASN:N	2.48	0.44
6:T:2889:PRO:HB2	6:T:2898:TRP:NE1	2.33	0.44
6:T:2923:LEU:HD11	6:T:2938:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:3433:ASN:OD1	6:T:3434:VAL:N	2.51	0.44
1:A:213:LYS:HA	1:A:217:CYS:SG	2.57	0.43
2:B:158:VAL:HG22	2:B:167:VAL:HG22	2.00	0.43
2:B:434:SER:HA	4:E:251:ILE:CD1	2.48	0.43
3:D:277:ILE:HD12	5:F:577:TYR:CZ	2.52	0.43
3:D:597:PHE:HE1	5:F:639:ARG:NE	2.16	0.43
3:D:615:LEU:HD12	3:D:619:ARG:HH12	1.83	0.43
5:F:540:ASP:OD1	5:F:544:ASN:HB3	2.18	0.43
5:F:559:ASN:N	5:F:559:ASN:OD1	2.47	0.43
6:T:349:HIS:CD2	6:T:352:ARG:HH12	2.35	0.43
6:T:629:GLU:OE2	6:T:1717:GLN:CA	2.66	0.43
6:T:1889:PHE:C	6:T:1889:PHE:CD2	2.96	0.43
6:T:2607:LEU:HD21	6:T:2624:LYS:HE3	1.99	0.43
6:T:2783:VAL:HG12	6:T:2791:ARG:NE	2.33	0.43
6:T:2840:LYS:HE3	6:T:2840:LYS:HB2	1.80	0.43
6:T:3086:LEU:HD23	6:T:3104:ILE:HD13	1.99	0.43
1:A:241:GLU:HA	1:A:247:VAL:HA	2.00	0.43
1:A:255:PHE:C	1:A:258:PRO:HD2	2.43	0.43
2:B:416:SER:HA	2:B:448:ARG:NH1	2.32	0.43
4:E:169:ILE:HG21	4:E:204:LYS:HE2	2.00	0.43
6:T:116:ILE:O	6:T:120:LYS:HD3	2.18	0.43
6:T:981:LYS:N	6:T:2483:GLU:OE1	2.50	0.43
6:T:1890:CYS:SG	6:T:1891:TRP:N	2.90	0.43
6:T:1936:VAL:CG2	6:T:1939:ARG:HD3	2.44	0.43
6:T:2174:ASN:HB3	6:T:2175:LYS:CE	2.47	0.43
6:T:2191:LEU:HA	6:T:2194:CYS:SG	2.58	0.43
6:T:3464:PHE:HB3	6:T:3575:ASP:OD1	2.18	0.43
1:A:189:LEU:O	1:A:192:ILE:HG12	2.18	0.43
2:B:253:LYS:HE2	2:B:258:THR:HG22	2.00	0.43
3:D:76:ARG:HD2	3:D:77:GLY:N	2.33	0.43
3:D:294:SER:HB2	3:D:321:GLU:OE2	2.19	0.43
4:E:198:LEU:HA	4:E:201:LEU:HB3	2.01	0.43
5:F:609:LEU:N	5:F:613:ARG:HH21	2.16	0.43
6:T:942:SER:OG	6:T:943:HIS:N	2.52	0.43
6:T:1210:ARG:HA	6:T:1213:VAL:HG12	1.99	0.43
6:T:1300:ASN:HD21	6:T:1302:LYS:HB2	1.82	0.43
6:T:1473:LEU:N	6:T:1474:PRO:HD2	2.33	0.43
6:T:1738:ARG:HA	6:T:1738:ARG:HE	1.81	0.43
6:T:1913:ILE:HD12	6:T:1923:VAL:CG2	2.48	0.43
6:T:2022:SER:HB3	6:T:2025:HIS:HE1	1.82	0.43
6:T:3089:ALA:HB1	6:T:3097:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:3225:SER:HB3	6:T:3349:PHE:CE1	2.53	0.43
6:T:3685:ASN:CG	6:T:3687:GLN:HB3	2.43	0.43
1:A:98:PRO:HA	1:A:101:HIS:CD2	2.53	0.43
2:B:69:TYR:HE2	2:B:229:LEU:HD21	1.84	0.43
6:T:24:ARG:HE	6:T:74:LYS:HB2	1.82	0.43
6:T:591:MET:HB3	6:T:689:MET:HE1	1.99	0.43
6:T:688:PHE:O	6:T:692:GLN:NE2	2.51	0.43
6:T:1333:LEU:O	6:T:1336:PRO:HD2	2.18	0.43
6:T:1492:HIS:ND1	6:T:1494:LYS:HB2	2.34	0.43
6:T:1592:PHE:C	6:T:1595:PRO:HD2	2.44	0.43
6:T:3282:LYS:O	6:T:3285:THR:HG22	2.19	0.43
6:T:952:LEU:O	6:T:952:LEU:HD12	2.19	0.43
6:T:1043:LEU:HD11	6:T:1115:VAL:HG11	2.00	0.43
6:T:1175:SER:HA	6:T:1178:ILE:HG22	2.00	0.43
6:T:1378:LEU:O	6:T:1382:ILE:HG12	2.18	0.43
6:T:1413:ILE:HD11	6:T:1458:THR:HG21	1.99	0.43
6:T:1757:LYS:HD3	6:T:1802:VAL:HG22	2.00	0.43
6:T:1872:ILE:HD12	6:T:1912:PHE:HD2	1.84	0.43
6:T:2245:GLN:NE2	6:T:2245:GLN:CA	2.73	0.43
6:T:2621:HIS:CE1	6:T:2622:LEU:HG	2.54	0.43
6:T:2746:LEU:H	6:T:2746:LEU:HD23	1.83	0.43
6:T:2774:ASP:OD1	6:T:2775:ALA:N	2.49	0.43
6:T:3626:PRO:HA	6:T:3629:GLN:HG2	2.00	0.43
2:B:255:LEU:O	2:B:259:LYS:NZ	2.48	0.43
3:D:393:ASP:HA	3:D:396:THR:HG22	2.00	0.43
3:D:537:LYS:HG3	3:D:538:GLU:H	1.83	0.43
6:T:381:PHE:CG	6:T:1859:LEU:HD21	2.53	0.43
6:T:570:LEU:C	6:T:572:LEU:H	2.26	0.43
6:T:1091:SER:O	6:T:1091:SER:OG	2.33	0.43
6:T:1107:LEU:HD23	6:T:1107:LEU:HA	1.83	0.43
6:T:1962:THR:N	6:T:1963:PRO:CD	2.81	0.43
6:T:2244:THR:CG2	6:T:2274:LEU:HD22	2.48	0.43
6:T:2451:LEU:HD12	6:T:2451:LEU:HA	1.79	0.43
6:T:2842:LEU:O	6:T:2845:GLY:N	2.52	0.43
1:A:314:GLN:HE22	1:A:328:LYS:HA	1.84	0.43
2:B:47:TYR:HH	2:B:66:ARG:HH21	1.63	0.43
2:B:199:GLU:N	2:B:200:PRO:HD2	2.34	0.43
2:B:441:THR:HG22	3:D:68:PHE:HA	2.01	0.43
2:B:474:GLU:O	2:B:478:VAL:HG12	2.19	0.43
3:D:379:TYR:OH	3:D:532:THR:HG21	2.19	0.43
6:T:1448:MET:CE	6:T:1456:ILE:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1483:LYS:N	6:T:1484:PRO:CD	2.82	0.43
6:T:1546:GLN:OE1	6:T:1546:GLN:HA	2.19	0.43
6:T:2204:GLU:H	6:T:2204:GLU:HG3	1.63	0.43
6:T:2282:PHE:HE1	6:T:2335:THR:CB	2.31	0.43
6:T:3111:ASP:OD1	6:T:3111:ASP:N	2.48	0.43
2:B:162:HIS:HB2	7:B:501:ATP:O3'	2.19	0.43
5:F:581:LEU:HD11	5:F:613:ARG:HA	2.01	0.43
6:T:23:SER:HA	6:T:27:THR:HG23	2.01	0.43
6:T:80:LEU:HA	6:T:83:PHE:HB2	2.00	0.43
6:T:341:SER:OG	6:T:344:ARG:HB2	2.18	0.43
6:T:913:PHE:HZ	6:T:917:ILE:HD12	1.83	0.43
6:T:1075:GLN:NE2	6:T:2491:ILE:O	2.46	0.43
6:T:1300:ASN:O	6:T:1303:VAL:HG12	2.18	0.43
6:T:1377:LEU:O	6:T:1380:GLU:HG3	2.19	0.43
6:T:1497:VAL:N	6:T:1498:PRO:CD	2.81	0.43
6:T:1703:LEU:HD23	6:T:1703:LEU:O	2.18	0.43
6:T:1932:ARG:HE	6:T:1933:SER:H	1.67	0.43
6:T:2238:MET:SD	6:T:2238:MET:C	3.02	0.43
6:T:2387:GLU:HB3	6:T:2390:LEU:HB3	2.01	0.43
6:T:2482:ARG:HD2	6:T:2539:SER:HB2	2.01	0.43
6:T:2580:VAL:HA	6:T:2583:ILE:HG22	2.00	0.43
6:T:2828:TRP:CD1	6:T:2828:TRP:C	2.96	0.43
6:T:3095:SER:O	6:T:3096:LYS:HE2	2.18	0.43
6:T:3178:PHE:HA	6:T:3181:ILE:HD12	2.00	0.43
6:T:3267:ARG:NH1	6:T:3498:ASP:OD2	2.49	0.43
2:B:86:ALA:O	2:B:89:GLN:HB3	2.19	0.43
3:D:44:TYR:HD1	3:D:44:TYR:HA	1.71	0.43
3:D:600:LEU:HD13	3:D:600:LEU:HA	1.82	0.43
6:T:6:GLN:NE2	6:T:43:ASP:OD2	2.52	0.43
6:T:635:LYS:HB2	6:T:701:ILE:HD12	2.01	0.43
6:T:1541:GLN:OE1	6:T:1541:GLN:HA	2.18	0.43
6:T:2383:GLU:OE1	6:T:2383:GLU:N	2.52	0.43
6:T:2888:LEU:HD12	6:T:2888:LEU:HA	1.92	0.43
6:T:3414:ARG:NH2	6:T:3417:GLU:OE1	2.51	0.43
3:D:537:LYS:HG3	3:D:538:GLU:N	2.34	0.43
5:F:637:LYS:NZ	5:F:655:ASN:HB3	2.34	0.43
6:T:429:LEU:O	6:T:433:ILE:HG13	2.19	0.43
6:T:776:PHE:HB3	6:T:779:ILE:CG2	2.48	0.43
6:T:844:GLN:N	6:T:844:GLN:OE1	2.52	0.43
6:T:896:GLN:HA	6:T:899:ARG:HD2	2.01	0.43
6:T:1104:ASN:HB3	6:T:1170:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1346:PRO:O	6:T:1349:MET:N	2.52	0.43
6:T:1588:LEU:O	6:T:1588:LEU:HG	2.19	0.43
6:T:1969:TRP:HA	6:T:1972:ARG:HB2	2.01	0.43
6:T:2274:LEU:C	6:T:2277:PRO:HD2	2.44	0.43
6:T:2637:ILE:O	6:T:2638:ASN:C	2.61	0.43
6:T:2770:ASN:OD1	6:T:2771:SER:N	2.52	0.43
1:A:150:GLY:HA2	1:A:293:LEU:HD12	2.01	0.42
2:B:418:PRO:HG3	3:D:75:ARG:HH12	1.83	0.42
3:D:287:LEU:HB2	4:E:265:GLU:OE1	2.18	0.42
3:D:533:GLU:H	3:D:533:GLU:CD	2.27	0.42
6:T:222:LYS:NZ	6:T:234:LEU:HD22	2.34	0.42
6:T:330:ILE:HD13	6:T:372:ASP:HB3	2.01	0.42
6:T:518:MET:CE	6:T:2317:ILE:HD13	2.48	0.42
6:T:570:LEU:O	6:T:571:LEU:HG	2.19	0.42
6:T:788:LEU:O	6:T:791:LEU:HB3	2.19	0.42
6:T:1518:ILE:HA	6:T:1521:LYS:HE2	2.01	0.42
6:T:1936:VAL:HG23	6:T:1939:ARG:NH1	2.34	0.42
6:T:3551:GLN:HB3	6:T:3581:VAL:HG12	2.01	0.42
2:B:129:LEU:HD23	2:B:129:LEU:HA	1.73	0.42
3:D:536:LYS:HD2	3:D:536:LYS:HA	1.76	0.42
3:D:601:LEU:HD23	3:D:601:LEU:HA	1.78	0.42
3:D:723:TRP:HE3	3:D:724:LEU:HD22	1.84	0.42
5:F:521:GLN:H	5:F:521:GLN:CD	2.27	0.42
6:T:3:LEU:HG	6:T:5:GLU:H	1.84	0.42
6:T:349:HIS:O	6:T:352:ARG:HG2	2.19	0.42
6:T:400:HIS:HB2	6:T:438:LEU:HD22	2.01	0.42
6:T:439:LEU:O	6:T:443:VAL:HG13	2.18	0.42
6:T:1011:ILE:HA	6:T:1014:ARG:HD3	2.01	0.42
6:T:1776:LYS:NZ	6:T:1778:LYS:HG3	2.33	0.42
6:T:1815:VAL:HG21	6:T:1870:ILE:CG1	2.49	0.42
6:T:1970:VAL:HG12	6:T:2003:PHE:CE2	2.54	0.42
6:T:3105:LEU:HD21	6:T:3133:TRP:HZ3	1.83	0.42
2:B:203:ILE:HA	2:B:274:TRP:CH2	2.55	0.42
2:B:472:LYS:HE2	2:B:476:GLU:HG3	2.01	0.42
3:D:308:LYS:NZ	4:E:281:LEU:HD21	2.34	0.42
3:D:374:LYS:O	3:D:378:LYS:HG3	2.19	0.42
4:E:198:LEU:O	4:E:202:LYS:HG2	2.19	0.42
6:T:1157:ILE:O	6:T:1161:ARG:HG3	2.19	0.42
6:T:1206:TYR:CE2	6:T:1253:PRO:HD2	2.54	0.42
6:T:1474:PRO:HG3	6:T:1511:ILE:HD13	2.00	0.42
6:T:1559:PHE:HB3	6:T:1599:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1564:PRO:HD3	6:T:1602:ARG:NH2	2.35	0.42
6:T:1600:LEU:N	6:T:1600:LEU:HD23	2.34	0.42
6:T:1673:PHE:HA	6:T:1676:MET:HG2	2.01	0.42
6:T:1930:LEU:CB	6:T:1946:LEU:HD21	2.48	0.42
6:T:2115:GLU:HB2	6:T:2116:LEU:HD23	2.00	0.42
6:T:2219:ALA:HB3	6:T:2222:VAL:CG1	2.50	0.42
6:T:2640:LEU:HD23	6:T:2640:LEU:HA	1.78	0.42
6:T:3240:THR:CG2	6:T:3243:GLU:H	2.31	0.42
6:T:3416:GLU:CD	6:T:3586:MET:H	2.26	0.42
1:A:361:GLU:O	1:A:365:SER:OG	2.26	0.42
3:D:25:LYS:O	3:D:28:LYS:N	2.50	0.42
5:F:627:LEU:O	5:F:628:GLU:HG3	2.18	0.42
6:T:3:LEU:HD23	6:T:3:LEU:H	1.84	0.42
6:T:72:GLU:OE1	6:T:76:ARG:NH2	2.53	0.42
6:T:471:TYR:CE2	6:T:590:LEU:HD22	2.54	0.42
6:T:719:LEU:HA	6:T:722:VAL:CG2	2.49	0.42
6:T:934:PRO:HD3	6:T:2825:LEU:HG	2.01	0.42
6:T:1039:TYR:HE1	6:T:2497:PRO:HB2	1.84	0.42
6:T:1671:ASP:HA	6:T:1674:ASN:HD22	1.84	0.42
6:T:1750:PHE:O	6:T:1750:PHE:CD1	2.70	0.42
6:T:1822:LYS:HB2	6:T:1822:LYS:HE3	1.82	0.42
6:T:2191:LEU:HD12	6:T:2194:CYS:SG	2.60	0.42
6:T:2707:TYR:O	6:T:2711:GLN:HG3	2.17	0.42
6:T:2825:LEU:HD12	6:T:2825:LEU:HA	1.85	0.42
6:T:3050:ASP:CG	6:T:3052:ASN:H	2.26	0.42
6:T:3142:THR:O	6:T:3145:SER:OG	2.18	0.42
6:T:3528:LYS:O	6:T:3532:THR:HG22	2.20	0.42
6:T:3583:THR:HG22	6:T:3584:LEU:N	2.33	0.42
2:B:47:TYR:HD2	2:B:54:LYS:HG3	1.84	0.42
2:B:254:THR:HG22	2:B:423:ARG:NH2	2.34	0.42
3:D:609:GLU:C	3:D:611:SER:H	2.27	0.42
3:D:619:ARG:HD3	6:T:2443:LEU:HD23	2.00	0.42
4:E:82:GLU:OE2	4:E:92:ARG:NH1	2.52	0.42
6:T:310:ILE:HD13	6:T:350:ALA:HB1	2.00	0.42
6:T:332:LEU:O	6:T:336:CYS:HB3	2.19	0.42
6:T:357:THR:OG1	6:T:360:LYS:HB2	2.19	0.42
6:T:466:ILE:HA	6:T:1716:LEU:CD2	2.49	0.42
6:T:913:PHE:CZ	6:T:917:ILE:HD12	2.54	0.42
6:T:1066:THR:H	6:T:3476:LYS:HZ2	1.67	0.42
6:T:1849:LEU:HD21	6:T:1893:PHE:HA	2.01	0.42
6:T:1860:PHE:HA	6:T:1863:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1902:LYS:HB3	6:T:1906:TYR:CE2	2.55	0.42
6:T:1919:PRO:CG	6:T:1922:VAL:HB	2.47	0.42
6:T:1987:GLN:HE21	6:T:2007:ILE:HG22	1.83	0.42
6:T:2022:SER:HB3	6:T:2025:HIS:CE1	2.55	0.42
6:T:2365:ILE:HG13	6:T:2366:PHE:H	1.84	0.42
6:T:2620:PRO:O	6:T:2621:HIS:CG	2.72	0.42
6:T:2892:TRP:HA	6:T:3434:VAL:HG23	2.02	0.42
6:T:2936:ALA:HB3	6:T:2938:ARG:NH2	2.34	0.42
6:T:3079:SER:HA	6:T:3082:ILE:HG22	2.01	0.42
6:T:3422:LEU:HD12	6:T:3666:PHE:HB2	2.01	0.42
1:A:130:PRO:O	1:A:359:LYS:N	2.52	0.42
3:D:74:ILE:C	3:D:76:ARG:H	2.27	0.42
3:D:270:PHE:O	5:F:587:GLY:N	2.32	0.42
3:D:368:TRP:CD2	3:D:571:GLU:CD	2.98	0.42
6:T:56:LEU:HB2	6:T:102:PHE:HZ	1.84	0.42
6:T:58:GLN:HG2	6:T:79:MET:HG2	2.01	0.42
6:T:81:ASP:HA	6:T:84:ASN:HD21	1.83	0.42
6:T:1140:LEU:HB2	6:T:2493:CYS:O	2.20	0.42
6:T:1654:ASN:HB3	6:T:1665:PHE:CZ	2.55	0.42
6:T:2214:MET:HA	6:T:2217:ILE:HG22	2.01	0.42
6:T:2444:GLU:HG3	6:T:2445:ARG:H	1.85	0.42
6:T:3137:ILE:HG23	6:T:3138:PRO:HD3	2.02	0.42
6:T:3137:ILE:HA	6:T:3140:LEU:HD12	2.01	0.42
2:B:227:LYS:HD3	2:B:227:LYS:HA	1.78	0.42
6:T:407:GLN:O	6:T:411:ILE:HG12	2.20	0.42
6:T:956:ASN:HD21	6:T:2843:LEU:CB	2.25	0.42
6:T:987:GLU:OE1	6:T:987:GLU:N	2.53	0.42
6:T:1456:ILE:HD12	6:T:1502:ALA:HB2	2.01	0.42
6:T:1830:LYS:C	6:T:1832:LYS:HE3	2.45	0.42
6:T:2369:VAL:HA	6:T:2372:LYS:HD3	2.02	0.42
6:T:2959:MET:HG2	6:T:2962:VAL:HG12	2.02	0.42
6:T:3081:ALA:HB1	6:T:3085:TYR:CE1	2.54	0.42
6:T:3326:ASP:OD2	6:T:3382:ARG:NH1	2.47	0.42
1:A:107:GLU:OE2	1:A:111:ASN:ND2	2.52	0.42
3:D:59:ASN:HA	5:F:568:SER:O	2.19	0.42
3:D:74:ILE:HD12	3:D:74:ILE:HA	1.95	0.42
3:D:309:ALA:HB3	6:T:2681:ARG:NH2	2.34	0.42
3:D:623:TYR:HB2	3:D:626:ARG:NE	2.27	0.42
4:E:262:LYS:O	4:E:266:MET:HG3	2.20	0.42
6:T:618:LEU:H	6:T:618:LEU:HD12	1.85	0.42
6:T:1416:ILE:HG21	6:T:1459:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1449:LEU:CD1	6:T:1484:PRO:HB2	2.48	0.42
6:T:1487:MET:HE2	6:T:1487:MET:N	2.34	0.42
6:T:1683:GLU:HG3	6:T:1686:LYS:H	1.84	0.42
6:T:2243:ILE:HD13	6:T:2243:ILE:HA	1.85	0.42
6:T:2262:VAL:HA	6:T:2265:MET:SD	2.59	0.42
6:T:2468:TRP:CD1	6:T:2468:TRP:C	2.97	0.42
6:T:2474:GLN:OE1	6:T:2546:ILE:HG23	2.19	0.42
6:T:2641:GLU:CD	6:T:3545:ARG:HH12	2.28	0.42
6:T:3464:PHE:CB	6:T:3575:ASP:HA	2.49	0.42
6:T:3623:ARG:NH2	6:T:3744:PHE:O	2.42	0.42
2:B:243:LYS:HA	2:B:247:CYS:SG	2.60	0.42
6:T:88:MET:HE3	6:T:88:MET:HB3	1.82	0.42
6:T:218:MET:HA	6:T:221:PHE:CD2	2.55	0.42
6:T:683:MET:O	6:T:686:LEU:HG	2.20	0.42
6:T:758:THR:O	6:T:762:LEU:HD23	2.20	0.42
6:T:849:ALA:C	6:T:851:LEU:N	2.78	0.42
6:T:879:LEU:HD13	6:T:879:LEU:HA	1.90	0.42
6:T:1342:LEU:HA	6:T:1342:LEU:HD12	1.78	0.42
6:T:1617:LEU:HD12	6:T:1620:LEU:HD23	2.02	0.42
6:T:1814:GLU:HA	6:T:1817:THR:HG22	2.02	0.42
6:T:1854:LEU:C	6:T:1854:LEU:CD2	2.85	0.42
6:T:2259:LEU:HD23	6:T:2259:LEU:C	2.44	0.42
6:T:2316:TYR:CE2	6:T:2348:PHE:HD2	2.38	0.42
6:T:2760:LEU:HD11	6:T:2790:ARG:HH21	1.84	0.42
1:A:375:PHE:CD1	3:D:380:LYS:HB2	2.54	0.42
2:B:431:ILE:HG23	2:B:432:LEU:N	2.35	0.42
5:F:583:GLU:OE1	5:F:583:GLU:N	2.52	0.42
6:T:72:GLU:CB	6:T:76:ARG:HE	2.33	0.42
6:T:295:ILE:O	6:T:299:ILE:HG12	2.20	0.42
6:T:1821:LEU:CD1	6:T:1824:TYR:HB2	2.50	0.42
6:T:2195:ILE:CG2	6:T:2239:LEU:HD22	2.50	0.42
6:T:2443:LEU:HD11	6:T:2453:TYR:CD2	2.55	0.42
6:T:2523:VAL:O	6:T:2527:ILE:HG12	2.20	0.42
6:T:2546:ILE:HA	6:T:2546:ILE:HD13	1.86	0.42
1:A:12:ASN:HD21	1:A:71:ILE:HG21	1.85	0.41
1:A:238:LYS:HE3	1:A:238:LYS:HB3	1.93	0.41
2:B:16:ALA:CB	2:B:107:PRO:HG2	2.50	0.41
3:D:537:LYS:HG3	3:D:538:GLU:OE1	2.20	0.41
5:F:653:MET:HE2	5:F:653:MET:HB3	1.85	0.41
6:T:474:ARG:HA	6:T:474:ARG:HD2	1.89	0.41
6:T:700:GLU:OE1	6:T:1587:GLN:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1155:TYR:CD2	6:T:1160:VAL:HG21	2.55	0.41
6:T:1396:ILE:HG13	6:T:1397:GLN:H	1.84	0.41
6:T:1448:MET:HA	6:T:1456:ILE:HG22	2.02	0.41
6:T:1454:GLU:HA	6:T:1457:ASN:HD21	1.85	0.41
6:T:1543:LEU:CB	6:T:1591:PRO:HG3	2.50	0.41
6:T:1568:MET:O	6:T:1568:MET:SD	2.78	0.41
6:T:1792:SER:HA	6:T:1794:LYS:NZ	2.34	0.41
2:B:49:ALA:N	2:B:68:ASP:OD2	2.53	0.41
2:B:281:ASP:OD2	2:B:283:GLU:HB3	2.20	0.41
2:B:405:ALA:O	2:B:437:PHE:HA	2.20	0.41
3:D:70:LYS:NZ	3:D:539:LEU:H	2.18	0.41
3:D:258:TYR:CZ	5:F:553:LYS:HB2	2.54	0.41
3:D:650:TRP:CZ3	3:D:699:ARG:HG2	2.55	0.41
4:E:180:ASP:HB3	4:E:182:ARG:NE	2.35	0.41
6:T:470:SER:HA	6:T:473:ASN:HD21	1.85	0.41
6:T:482:TYR:HD1	6:T:647:PHE:CE1	2.38	0.41
6:T:965:ASP:C	6:T:966:LEU:HD22	2.45	0.41
6:T:1574:LEU:HD22	6:T:1623:PHE:CE2	2.49	0.41
6:T:3009:THR:HG23	6:T:3010:ASN:H	1.86	0.41
3:D:348:PHE:H	4:E:236:ARG:NH1	2.19	0.41
6:T:611:TYR:OH	6:T:1584:LEU:O	2.37	0.41
6:T:1615:MET:HE3	6:T:1651:TYR:CE1	2.55	0.41
6:T:1881:GLU:CD	6:T:1881:GLU:N	2.73	0.41
6:T:2279:MET:HE2	6:T:2332:PHE:HB2	2.01	0.41
6:T:2571:ILE:HD12	6:T:2571:ILE:HA	1.95	0.41
6:T:3295:LYS:HG3	6:T:3317:TRP:CZ2	2.56	0.41
1:A:318:THR:HA	1:A:327:VAL:HG21	2.02	0.41
1:A:351:THR:O	1:A:354:GLN:HG2	2.21	0.41
6:T:50:ALA:O	6:T:53:PRO:HD2	2.20	0.41
6:T:914:ASP:HB2	6:T:915:PRO:HD3	2.02	0.41
6:T:1046:ALA:O	6:T:1050:ILE:HG12	2.20	0.41
6:T:1601:ASN:HA	6:T:1604:HIS:CE1	2.54	0.41
6:T:1684:TRP:CE3	6:T:1684:TRP:O	2.72	0.41
6:T:1912:PHE:C	6:T:1912:PHE:HD1	2.27	0.41
6:T:1932:ARG:HE	6:T:1932:ARG:HA	1.85	0.41
6:T:2325:LEU:CD1	6:T:2328:SER:HB3	2.46	0.41
6:T:2999:LEU:HD23	6:T:2999:LEU:O	2.21	0.41
6:T:3020:ALA:HB2	6:T:3049:ILE:HG21	2.02	0.41
6:T:3322:GLU:HG3	6:T:3382:ARG:HD3	2.01	0.41
2:B:56:ILE:H	2:B:56:ILE:HD12	1.85	0.41
4:E:292:THR:HB	4:E:295:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:560:VAL:HB	5:F:561:PRO:CD	2.51	0.41
6:T:464:LEU:HA	6:T:467:ILE:HG22	2.02	0.41
6:T:854:GLU:HG2	6:T:855:ARG:H	1.85	0.41
6:T:1529:TRP:HA	6:T:1529:TRP:CE3	2.56	0.41
6:T:1565:GLN:HE21	6:T:1565:GLN:HB2	1.55	0.41
6:T:1591:PRO:HG2	6:T:1592:PHE:CD1	2.55	0.41
6:T:1651:TYR:CD1	6:T:1665:PHE:HB3	2.55	0.41
6:T:2573:LYS:C	6:T:2575:GLU:N	2.78	0.41
6:T:2852:PHE:O	6:T:2855:ALA:HB3	2.20	0.41
6:T:3365:ASN:OD1	6:T:3365:ASN:C	2.62	0.41
1:A:209:VAL:HA	1:A:212:ILE:HD12	2.03	0.41
1:A:272:ALA:H	2:B:60:GLN:NE2	2.19	0.41
1:A:299:MET:HE2	1:A:299:MET:HB2	1.83	0.41
2:B:64:ILE:O	2:B:66:ARG:NH1	2.51	0.41
4:E:185:LEU:HD23	4:E:185:LEU:H	1.84	0.41
4:E:246:ARG:HE	4:E:246:ARG:HB2	1.54	0.41
6:T:132:ILE:HD12	6:T:134:GLN:HG2	2.01	0.41
6:T:840:GLN:OE1	6:T:878:PHE:HB3	2.20	0.41
6:T:859:VAL:O	6:T:863:ILE:HG12	2.21	0.41
6:T:913:PHE:CE1	6:T:917:ILE:HB	2.56	0.41
6:T:934:PRO:HG3	6:T:2825:LEU:O	2.21	0.41
6:T:1057:ILE:HG22	6:T:1058:GLU:N	2.36	0.41
6:T:1461:GLU:C	6:T:1461:GLU:CD	2.88	0.41
6:T:1848:ILE:HG21	6:T:1852:ASP:N	2.31	0.41
6:T:2204:GLU:HA	6:T:2207:GLN:NE2	2.35	0.41
6:T:2320:LEU:HD21	6:T:2355:MET:O	2.21	0.41
6:T:3140:LEU:O	6:T:3144:LEU:HG	2.20	0.41
1:A:323:SER:H	2:B:271:GLU:CD	2.29	0.41
2:B:100:LEU:HD21	2:B:106:ILE:HD13	2.03	0.41
2:B:145:CYS:O	2:B:455:GLY:HA3	2.21	0.41
2:B:290:GLU:OE1	2:B:423:ARG:NH1	2.39	0.41
2:B:432:LEU:HD23	2:B:432:LEU:HA	1.95	0.41
3:D:617:LYS:HD2	3:D:617:LYS:HA	1.76	0.41
5:F:531:ASP:HA	5:F:534:VAL:HG12	2.02	0.41
6:T:129:PHE:CD1	6:T:132:ILE:HD11	2.55	0.41
6:T:464:LEU:O	6:T:468:ILE:HG12	2.19	0.41
6:T:1328:HIS:O	6:T:1328:HIS:ND1	2.54	0.41
6:T:1342:LEU:HB2	6:T:1377:LEU:HD11	2.02	0.41
6:T:1617:LEU:HD12	6:T:1620:LEU:CD2	2.49	0.41
6:T:1703:LEU:CD1	6:T:1753:SER:HB2	2.51	0.41
6:T:1798:ALA:HB3	6:T:1799:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1876:PRO:HA	6:T:1883:LYS:CE	2.50	0.41
6:T:2315:LEU:C	6:T:2315:LEU:CD1	2.93	0.41
6:T:2349:LEU:O	6:T:2353:VAL:HG13	2.20	0.41
1:A:143:TYR:CE1	3:D:391:ILE:HG13	2.56	0.41
3:D:396:THR:HG23	3:D:397:TYR:CD1	2.56	0.41
4:E:198:LEU:HD23	4:E:198:LEU:H	1.85	0.41
6:T:586:LEU:O	6:T:590:LEU:HG	2.21	0.41
6:T:611:TYR:CZ	6:T:1585:ARG:HB3	2.55	0.41
6:T:623:SER:C	6:T:624:ARG:HD2	2.46	0.41
6:T:1049:SER:HA	6:T:1052:LEU:HG	2.03	0.41
6:T:1832:LYS:N	6:T:1832:LYS:CE	2.84	0.41
6:T:2768:ASP:HB2	6:T:2770:ASN:OD1	2.20	0.41
6:T:3172:ARG:O	6:T:3173:THR:C	2.64	0.41
6:T:3623:ARG:NH1	6:T:3625:THR:HB	2.35	0.41
1:A:70:PRO:HB3	1:A:78:ASN:HB3	2.02	0.41
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.90	0.41
2:B:64:ILE:HB	2:B:66:ARG:NH1	2.36	0.41
2:B:75:ILE:HD13	2:B:75:ILE:HA	1.87	0.41
2:B:116:ASN:OD1	2:B:120:ASN:HB3	2.21	0.41
2:B:121:ARG:O	2:B:124:SER:OG	2.29	0.41
3:D:68:PHE:CE2	3:D:69:LEU:HG	2.56	0.41
3:D:344:GLN:O	5:F:538:LEU:HD13	2.20	0.41
3:D:539:LEU:HD23	3:D:539:LEU:HA	1.78	0.41
3:D:558:THR:HB	3:D:561:GLN:CD	2.46	0.41
3:D:658:LEU:HD13	3:D:696:CYS:SG	2.61	0.41
4:E:173:PHE:HA	4:E:176:CYS:CB	2.51	0.41
4:E:233:GLU:O	4:E:237:LYS:HG2	2.21	0.41
6:T:5:GLU:O	6:T:8:GLU:HG3	2.20	0.41
6:T:5:GLU:O	6:T:9:GLN:HG2	2.20	0.41
6:T:342:SER:HA	6:T:345:LYS:HG3	2.03	0.41
6:T:706:LEU:HA	6:T:709:VAL:HB	2.03	0.41
6:T:744:LEU:HD12	6:T:766:PHE:CZ	2.56	0.41
6:T:1001:LEU:HD23	6:T:1001:LEU:HA	1.82	0.41
6:T:1070:ARG:NH1	6:T:3534:LEU:HD13	2.35	0.41
6:T:1116:ASN:OD1	6:T:2500:LEU:HB3	2.21	0.41
6:T:1291:ASP:OD1	6:T:1292:ILE:N	2.54	0.41
6:T:1495:LEU:HB3	6:T:1500:LEU:HD11	2.03	0.41
6:T:1513:TYR:O	6:T:1513:TYR:CD1	2.70	0.41
6:T:1635:GLU:OE1	6:T:1635:GLU:N	2.53	0.41
6:T:1662:VAL:HG21	6:T:1705:THR:HG23	2.02	0.41
6:T:1737:GLU:CD	6:T:1737:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1911:TYR:C	6:T:1911:TYR:CD2	2.98	0.41
6:T:1927:PHE:C	6:T:1927:PHE:CD1	2.99	0.41
6:T:2278:LEU:C	6:T:2278:LEU:CD1	2.85	0.41
6:T:3106:TRP:CH2	6:T:3689:ARG:HD2	2.55	0.41
6:T:3420:PHE:HA	6:T:3445:LEU:HD11	2.03	0.41
6:T:3431:SER:HB2	6:T:3442:GLN:OE1	2.21	0.41
6:T:3472:ASN:ND2	6:T:3482:PRO:HG2	2.33	0.41
6:T:3524:SER:OG	6:T:3525:ASN:N	2.53	0.41
6:T:3695:ASN:O	6:T:3699:ILE:HG12	2.20	0.41
6:T:1357:ILE:HD13	6:T:1374:LEU:HD13	2.02	0.41
6:T:1467:LEU:O	6:T:1467:LEU:HG	2.21	0.41
6:T:1473:LEU:N	6:T:1474:PRO:CD	2.83	0.41
6:T:1907:LEU:HD12	6:T:1945:SER:HB3	2.03	0.41
6:T:2450:ARG:HH12	6:T:2478:GLY:C	2.29	0.41
6:T:3004:ASP:OD1	6:T:3007:SER:OG	2.38	0.41
6:T:3045:THR:O	6:T:3049:ILE:HG12	2.21	0.41
6:T:3118:THR:OG1	6:T:3119:ASN:N	2.54	0.41
6:T:3265:PHE:O	6:T:3267:ARG:HG3	2.21	0.41
6:T:3562:MET:HE2	6:T:3562:MET:HB3	1.82	0.41
1:A:134:VAL:HG12	1:A:374:CYS:SG	2.61	0.40
2:B:235:ASN:HA	2:B:239:PHE:CD2	2.56	0.40
3:D:323:ARG:O	3:D:326:VAL:HG12	2.20	0.40
3:D:572:GLU:C	3:D:574:PRO:HD3	2.46	0.40
5:F:574:ARG:HD3	5:F:574:ARG:H	1.87	0.40
6:T:305:LEU:O	6:T:308:VAL:HG12	2.21	0.40
6:T:463:LEU:HA	6:T:466:ILE:HD12	2.03	0.40
6:T:473:ASN:HA	6:T:476:LYS:HB3	2.03	0.40
6:T:514:SER:O	6:T:518:MET:HG3	2.22	0.40
6:T:609:ASN:OD1	6:T:610:GLU:N	2.54	0.40
6:T:839:LEU:HD23	6:T:839:LEU:HA	1.86	0.40
6:T:983:ASN:ND2	6:T:2479:SER:OG	2.51	0.40
6:T:1129:PHE:CD2	6:T:1131:ILE:HG12	2.56	0.40
6:T:1698:MET:O	6:T:1698:MET:SD	2.79	0.40
6:T:2461:GLU:HG3	6:T:2592:HIS:HB3	2.03	0.40
6:T:2940:TYR:O	6:T:2942:GLU:N	2.54	0.40
1:A:131:ALA:HA	1:A:357:ILE:O	2.20	0.40
2:B:136:ALA:HB1	2:B:470:VAL:O	2.21	0.40
2:B:176:LEU:O	2:B:180:THR:HG23	2.21	0.40
2:B:255:LEU:HB2	2:B:290:GLU:HG2	2.03	0.40
3:D:556:GLU:N	3:D:557:LYS:HZ3	2.18	0.40
6:T:710:TYR:HA	6:T:713:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:763:ILE:HD13	6:T:763:ILE:HA	1.93	0.40
6:T:1669:MET:HE3	6:T:1698:MET:HG2	2.04	0.40
6:T:1703:LEU:HD11	6:T:1753:SER:HB2	2.03	0.40
6:T:2271:ILE:HG12	6:T:2274:LEU:CG	2.47	0.40
6:T:2571:ILE:HG13	6:T:2572:PRO:HD2	2.03	0.40
1:A:234:SER:O	1:A:234:SER:OG	2.33	0.40
1:A:262:PHE:CE2	1:A:312:ARG:HG2	2.56	0.40
2:B:177:SER:O	2:B:180:THR:OG1	2.21	0.40
6:T:218:MET:HA	6:T:221:PHE:CE2	2.57	0.40
6:T:405:GLU:H	6:T:445:ARG:NH2	2.19	0.40
6:T:1245:LEU:HD11	6:T:1261:GLU:HB3	2.03	0.40
6:T:1486:LEU:HD23	6:T:1486:LEU:HA	1.95	0.40
6:T:1744:LEU:HA	6:T:1744:LEU:HD13	1.84	0.40
6:T:2214:MET:HE3	6:T:2214:MET:HB3	1.98	0.40
6:T:2346:GLN:O	6:T:2350:ARG:HG2	2.21	0.40
6:T:2455:ILE:HD13	6:T:2455:ILE:HA	1.89	0.40
6:T:2963:CYS:O	6:T:2967:LEU:HD23	2.21	0.40
6:T:3266:PRO:HB2	6:T:3268:LYS:NZ	2.37	0.40
6:T:3434:VAL:HG22	6:T:3435:GLU:H	1.87	0.40
1:A:99:GLU:O	1:A:130:PRO:HD3	2.22	0.40
1:A:148:THR:HG21	3:D:392:LYS:HD2	2.03	0.40
2:B:59:GLU:O	2:B:62:ILE:HG22	2.21	0.40
2:B:152:ARG:CZ	2:B:440:LEU:HD11	2.51	0.40
2:B:428:LEU:HD12	2:B:437:PHE:CZ	2.57	0.40
3:D:668:ASN:O	3:D:672:ILE:HG13	2.21	0.40
6:T:718:GLY:O	6:T:722:VAL:HG23	2.22	0.40
6:T:1213:VAL:HA	6:T:1216:ILE:HG22	2.04	0.40
6:T:1615:MET:HB2	6:T:1650:PHE:CZ	2.57	0.40
6:T:1907:LEU:HD23	6:T:1907:LEU:O	2.20	0.40
6:T:1950:THR:N	6:T:1951:PRO:CD	2.84	0.40
6:T:1962:THR:OG1	6:T:1963:PRO:CD	2.69	0.40
6:T:1994:ASP:HA	6:T:1997:PHE:HD2	1.85	0.40
6:T:2138:VAL:O	6:T:2138:VAL:HG12	2.21	0.40
6:T:2348:PHE:HA	6:T:2351:LYS:HB2	2.03	0.40
6:T:2706:LEU:O	6:T:2709:VAL:HG12	2.21	0.40
6:T:2902:VAL:HG13	6:T:2946:VAL:HG12	2.03	0.40
6:T:3208:LEU:HA	6:T:3208:LEU:HD12	1.83	0.40
6:T:3522:VAL:HG21	6:T:3743:TRP:CD1	2.57	0.40
1:A:76:VAL:HG21	1:A:79:TRP:CE3	2.56	0.40
1:A:160:THR:CG2	1:A:178:ILE:HB	2.52	0.40
6:T:107:LEU:HD22	6:T:143:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:115:GLY:O	6:T:119:MET:HG2	2.21	0.40
6:T:1447:THR:O	6:T:1456:ILE:HG22	2.22	0.40
6:T:1883:LYS:HB3	6:T:1912:PHE:HZ	1.83	0.40
6:T:1895:LYS:H	6:T:1895:LYS:CD	2.34	0.40
6:T:1910:SER:HA	6:T:1913:ILE:HD11	2.02	0.40
6:T:2004:ILE:H	6:T:2004:ILE:HG13	1.67	0.40
6:T:2236:ILE:HD12	6:T:2263:LEU:CD2	2.52	0.40
6:T:2477:TYR:CD2	6:T:2542:ILE:HB	2.52	0.40
6:T:2681:ARG:HD2	6:T:2681:ARG:HA	1.83	0.40
6:T:3067:ARG:HH12	6:T:3075:ILE:HG21	1.85	0.40
6:T:3552:TYR:OH	6:T:3623:ARG:O	2.35	0.40
6:T:3659:LEU:C	6:T:3661:THR:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/372 (100%)	346 (94%)	24 (6%)	0	100	100
2	B	398/481 (83%)	365 (92%)	33 (8%)	0	100	100
3	D	448/982 (46%)	357 (80%)	91 (20%)	0	100	100
4	E	197/476 (41%)	174 (88%)	23 (12%)	0	100	100
5	F	120/832 (14%)	93 (78%)	26 (22%)	1 (1%)	16	52
6	T	3445/3744 (92%)	3069 (89%)	366 (11%)	10 (0%)	36	70
All	All	4978/6887 (72%)	4404 (88%)	563 (11%)	11 (0%)	44	75

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	T	1796	LEU

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Mol	Chain	Res	Type
6	T	1980	SER
5	F	542	PRO
6	T	1993	PRO
6	T	1206	TYR
6	T	3443	PHE
6	T	3539	GLU
6	T	2295	PRO
6	T	3655	PRO
6	T	1605	ASN
6	T	3264	PRO

5.3.2 Protein sidechains [i](#)

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	317/317 (100%)	317 (100%)	0	100	100
2	B	354/428 (83%)	354 (100%)	0	100	100
3	D	414/892 (46%)	413 (100%)	1 (0%)	87	87
4	E	184/441 (42%)	184 (100%)	0	100	100
5	F	114/769 (15%)	113 (99%)	1 (1%)	70	76
6	T	3188/3452 (92%)	3117 (98%)	71 (2%)	45	65
All	All	4571/6299 (73%)	4498 (98%)	73 (2%)	54	70

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	78	ILE
5	F	572	ILE
6	T	310	ILE
6	T	727	LEU
6	T	1506	LEU
6	T	1509	LEU
6	T	1534	VAL
6	T	1543	LEU

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Mol	Chain	Res	Type
6	T	1558	ILE
6	T	1565	GLN
6	T	1586	LEU
6	T	1601	ASN
6	T	1609	GLU
6	T	1614	ASN
6	T	1616	THR
6	T	1635	GLU
6	T	1644	LEU
6	T	1660	VAL
6	T	1663	VAL
6	T	1669	MET
6	T	1678	ILE
6	T	1687	LYS
6	T	1692	ILE
6	T	1702	THR
6	T	1716	LEU
6	T	1718	LEU
6	T	1744	LEU
6	T	1750	PHE
6	T	1776	LYS
6	T	1779	GLN
6	T	1781	ASN
6	T	1790	VAL
6	T	1799	ARG
6	T	1826	VAL
6	T	1849	LEU
6	T	1854	LEU
6	T	1859	LEU
6	T	1877	GLU
6	T	1896	LEU
6	T	1900	LEU
6	T	1913	ILE
6	T	1918	PHE
6	T	1920	ILE
6	T	1927	PHE
6	T	1941	LEU
6	T	1949	LEU
6	T	1995	LEU
6	T	2002	LEU
6	T	2012	ASN
6	T	2031	LEU

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Mol	Chain	Res	Type
6	T	2092	LEU
6	T	2116	LEU
6	T	2122	ASN
6	T	2144	GLU
6	T	2163	ASN
6	T	2182	GLU
6	T	2189	ASN
6	T	2192	GLU
6	T	2194	CYS
6	T	2201	ASP
6	T	2206	LEU
6	T	2212	VAL
6	T	2217	ILE
6	T	2236	ILE
6	T	2243	ILE
6	T	2269	ASP
6	T	2271	ILE
6	T	2278	LEU
6	T	2311	LEU
6	T	2315	LEU
6	T	2325	LEU
6	T	2556	ILE
6	T	3068	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	73	HIS
1	A	87	HIS
1	A	128	ASN
1	A	137	GLN
1	A	161	HIS
1	A	353	GLN
1	A	372	HIS
2	B	37	GLN
2	B	60	GLN
2	B	95	GLN
2	B	103	ASN
2	B	120	ASN
2	B	191	ASN
2	B	234	ASN

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Mol	Chain	Res	Type
2	B	248	HIS
2	B	406	HIS
2	B	444	HIS
3	D	72	ASN
3	D	262	ASN
3	D	359	GLN
3	D	389	GLN
3	D	570	ASN
3	D	644	ASN
5	F	580	HIS
5	F	624	GLN
6	T	6	GLN
6	T	39	ASN
6	T	84	ASN
6	T	146	GLN
6	T	150	ASN
6	T	353	HIS
6	T	384	HIS
6	T	401	ASN
6	T	473	ASN
6	T	605	ASN
6	T	615	ASN
6	T	639	HIS
6	T	983	ASN
6	T	1060	ASN
6	T	1104	ASN
6	T	1105	ASN
6	T	1116	ASN
6	T	1234	GLN
6	T	1287	ASN
6	T	1300	ASN
6	T	1312	HIS
6	T	1316	ASN
6	T	1379	GLN
6	T	1457	ASN
6	T	1470	ASN
6	T	1493	GLN
6	T	1525	HIS
6	T	1546	GLN
6	T	1565	GLN
6	T	1571	ASN
6	T	1601	ASN

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Mol	Chain	Res	Type
6	T	1604	HIS
6	T	1659	GLN
6	T	1709	ASN
6	T	1768	HIS
6	T	1769	ASN
6	T	1780	ASN
6	T	1805	ASN
6	T	1838	HIS
6	T	1866	GLN
6	T	1903	GLN
6	T	1944	GLN
6	T	1977	ASN
6	T	1981	GLN
6	T	1987	GLN
6	T	1998	ASN
6	T	2009	HIS
6	T	2122	ASN
6	T	2174	ASN
6	T	2183	ASN
6	T	2188	GLN
6	T	2189	ASN
6	T	2200	HIS
6	T	2207	GLN
6	T	2245	GLN
6	T	2266	ASN
6	T	2418	GLN
6	T	2458	GLN
6	T	2592	HIS
6	T	2644	GLN
6	T	2646	ASN
6	T	2651	ASN
6	T	2704	GLN
6	T	2741	GLN
6	T	2811	GLN
6	T	2861	ASN
6	T	2869	ASN
6	T	2896	ASN
6	T	2957	HIS
6	T	2992	HIS
6	T	3041	GLN
6	T	3059	GLN
6	T	3064	ASN

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Mol	Chain	Res	Type
6	T	3073	ASN
6	T	3119	ASN
6	T	3139	GLN
6	T	3154	HIS
6	T	3232	GLN
6	T	3357	GLN
6	T	3367	HIS
6	T	3385	HIS
6	T	3421	GLN
6	T	3444	ASN
6	T	3515	ASN
6	T	3537	GLN
6	T	3629	GLN
6	T	3657	ASN
6	T	3679	HIS
6	T	3695	ASN

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](#)

1 ligand is modelled in this entry.

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	ATP	B	501	-	32,33,33	1.30	5 (15%)	48,52,52	1.77	11 (22%)

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	ATP	B	501	-	-	3/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ATP	C5-C4	4.34	1.46	1.39
7	B	501	ATP	C5-C6	2.51	1.48	1.41
7	B	501	ATP	C5-N7	-2.46	1.34	1.39
7	B	501	ATP	C4-N9	-2.32	1.32	1.37
7	B	501	ATP	C8-N7	2.09	1.35	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	ATP	C5-C4-N3	-5.66	118.93	126.72
7	B	501	ATP	N3-C4-N9	4.60	135.00	127.17
7	B	501	ATP	C2-N3-C4	3.58	120.57	111.83
7	B	501	ATP	C4-C5-N7	-3.28	106.83	110.58
7	B	501	ATP	N3-C2-N1	-3.05	123.97	128.58
7	B	501	ATP	C4-N9-C8	3.02	108.91	105.74
7	B	501	ATP	C3'-C2'-C1'	2.38	105.97	101.46
7	B	501	ATP	C5-N7-C8	2.37	107.18	103.45
7	B	501	ATP	C2'-C1'-N9	-2.37	107.42	113.30
7	B	501	ATP	N9-C8-N7	-2.07	111.01	113.94
7	B	501	ATP	O2B-PB-O1B	2.06	122.05	112.44

There are no chirality outliers.

All (3) torsion outliers are listed below:

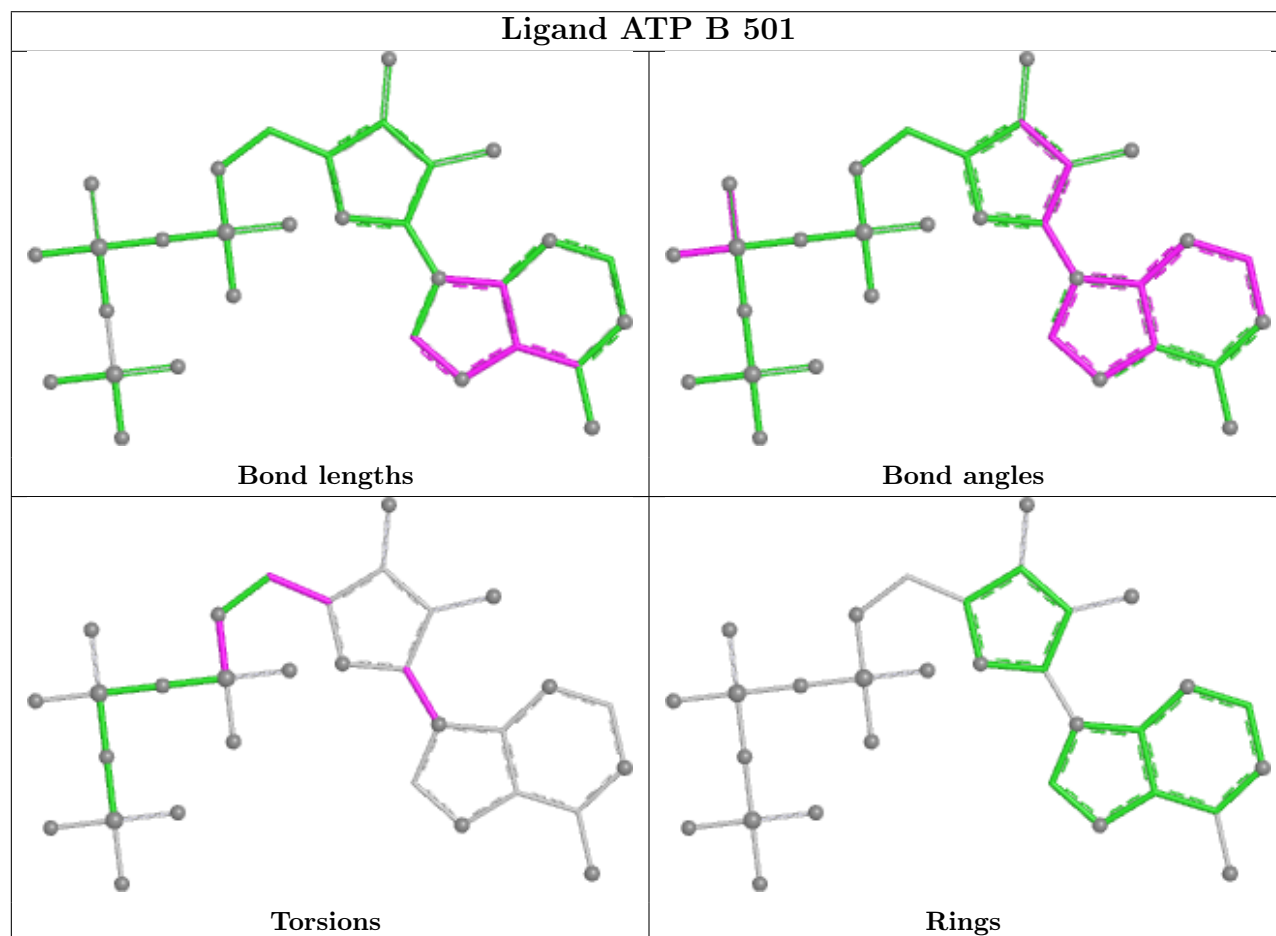
Mol	Chain	Res	Type	Atoms
7	B	501	ATP	C5'-O5'-PA-O1A
7	B	501	ATP	C2'-C1'-N9-C8
7	B	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	ATP	5	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

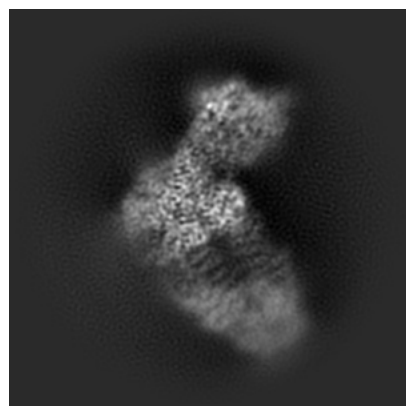
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33796. These allow visual inspection of the internal detail of the map and identification of artifacts.

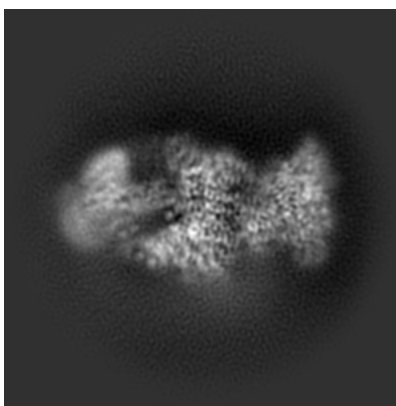
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

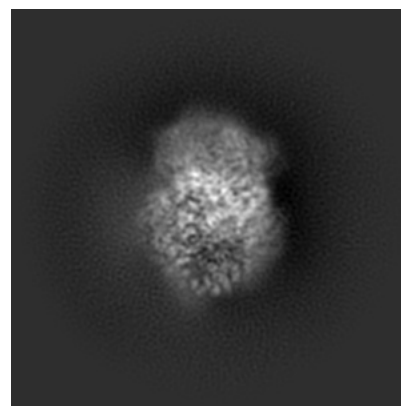
6.1.1 Primary map



X

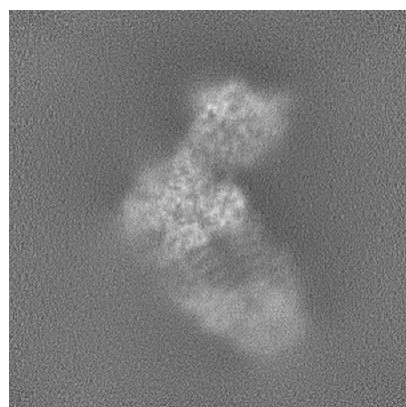


Y

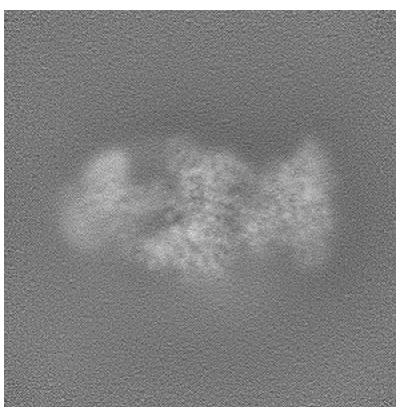


Z

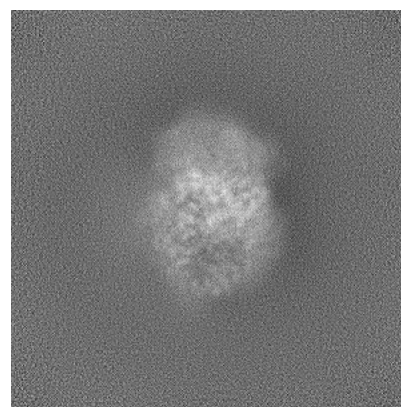
6.1.2 Raw map



X



Y

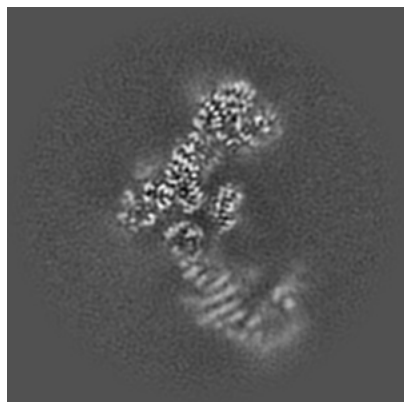


Z

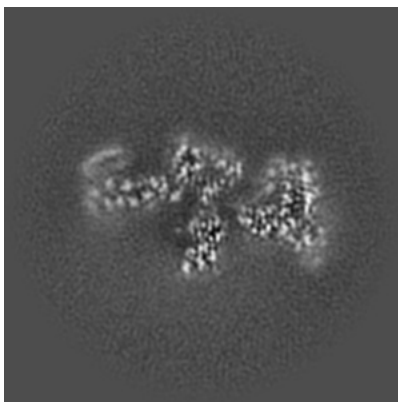
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

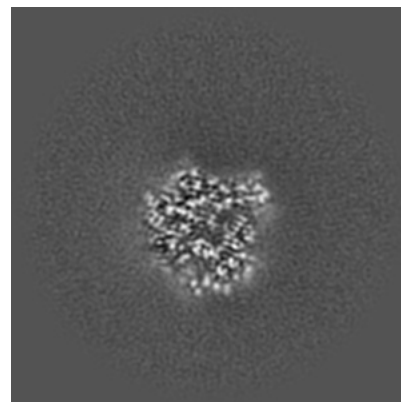
6.2.1 Primary map



X Index: 250

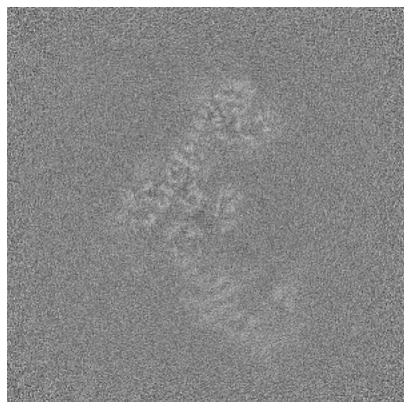


Y Index: 250

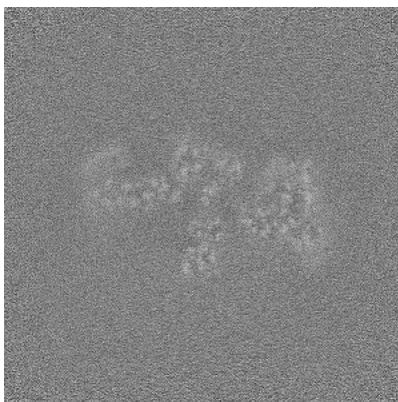


Z Index: 250

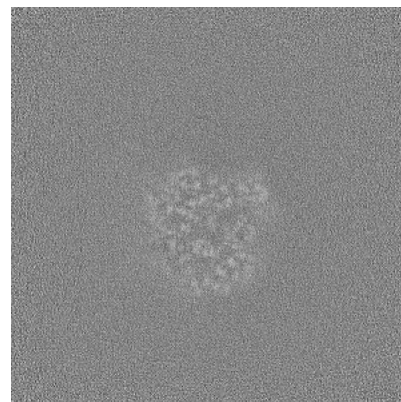
6.2.2 Raw map



X Index: 250



Y Index: 250

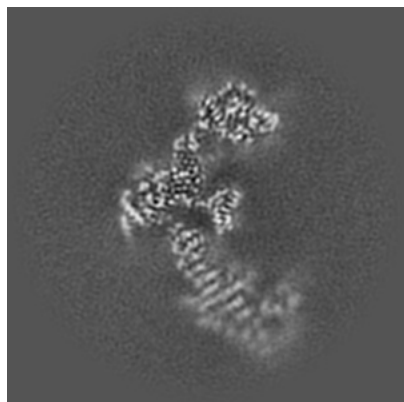


Z Index: 250

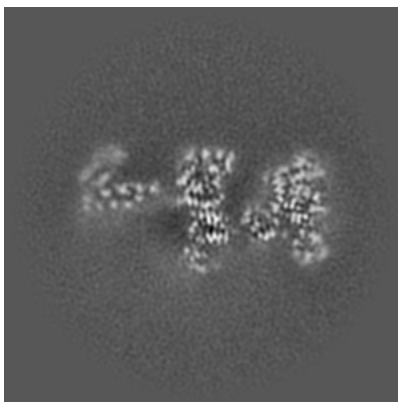
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

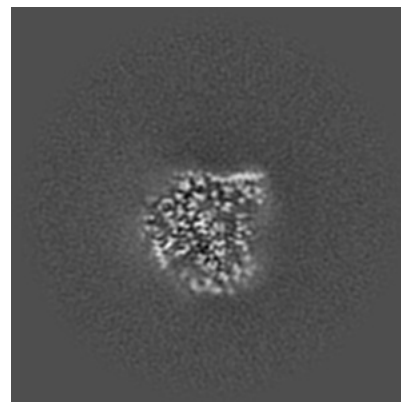
6.3.1 Primary map



X Index: 256

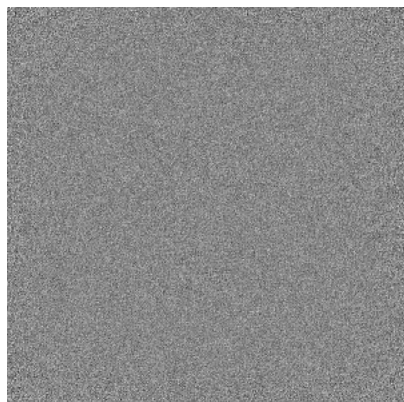


Y Index: 264

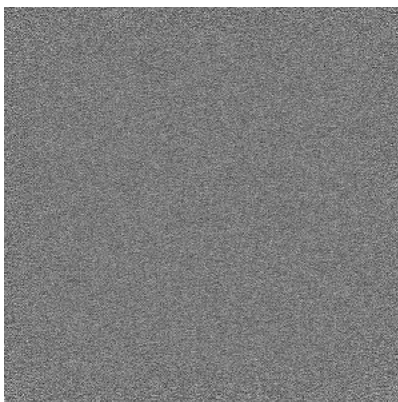


Z Index: 257

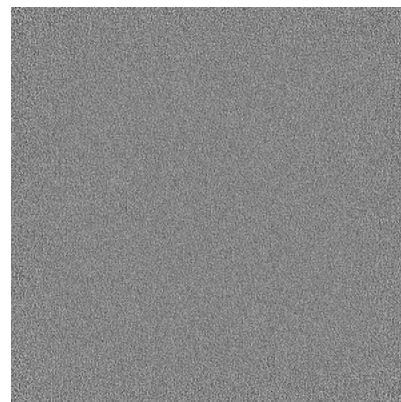
6.3.2 Raw map



X Index: 0



Y Index: 0

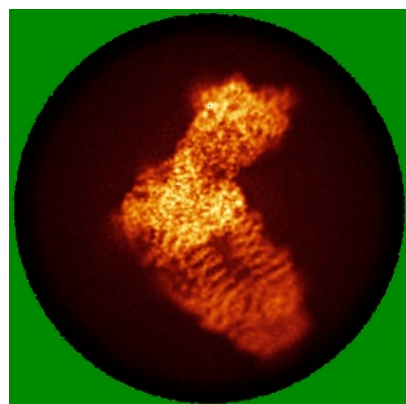


Z Index: 0

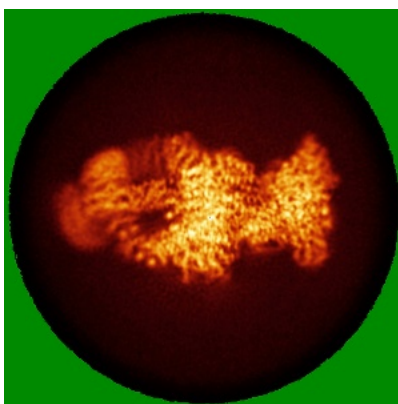
The images above show the largest variance slices of the map in three orthogonal directions.

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

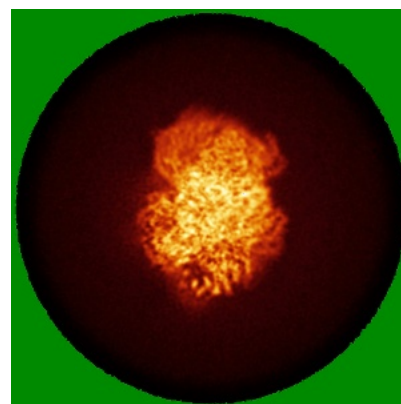
6.4.1 Primary map



X

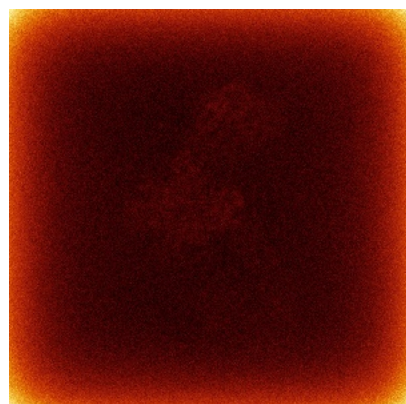


Y

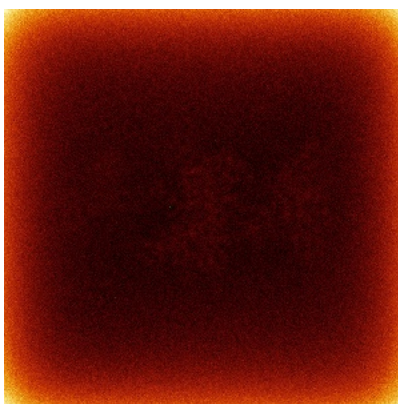


Z

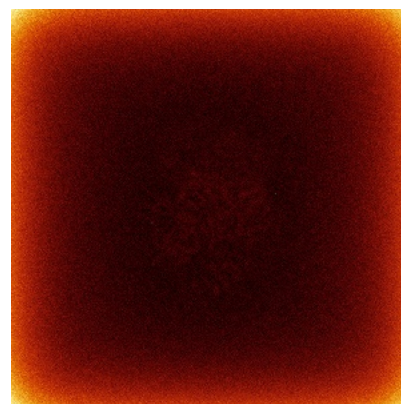
6.4.2 Raw map



X



Y

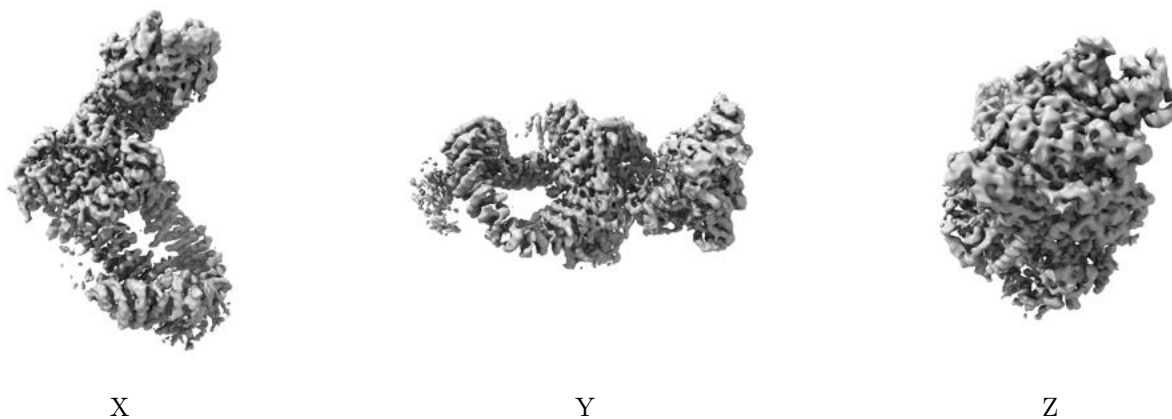


Z

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.

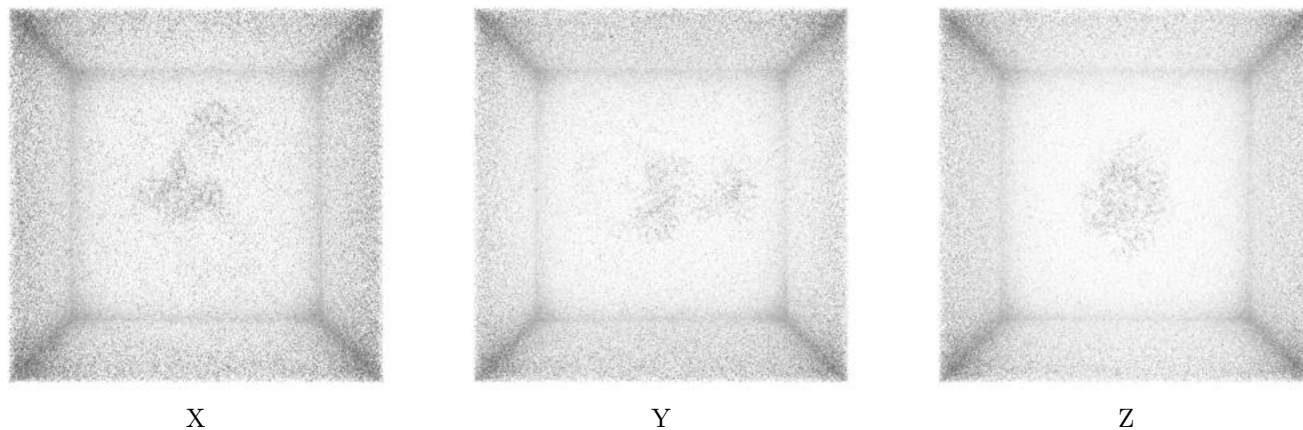
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0396. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

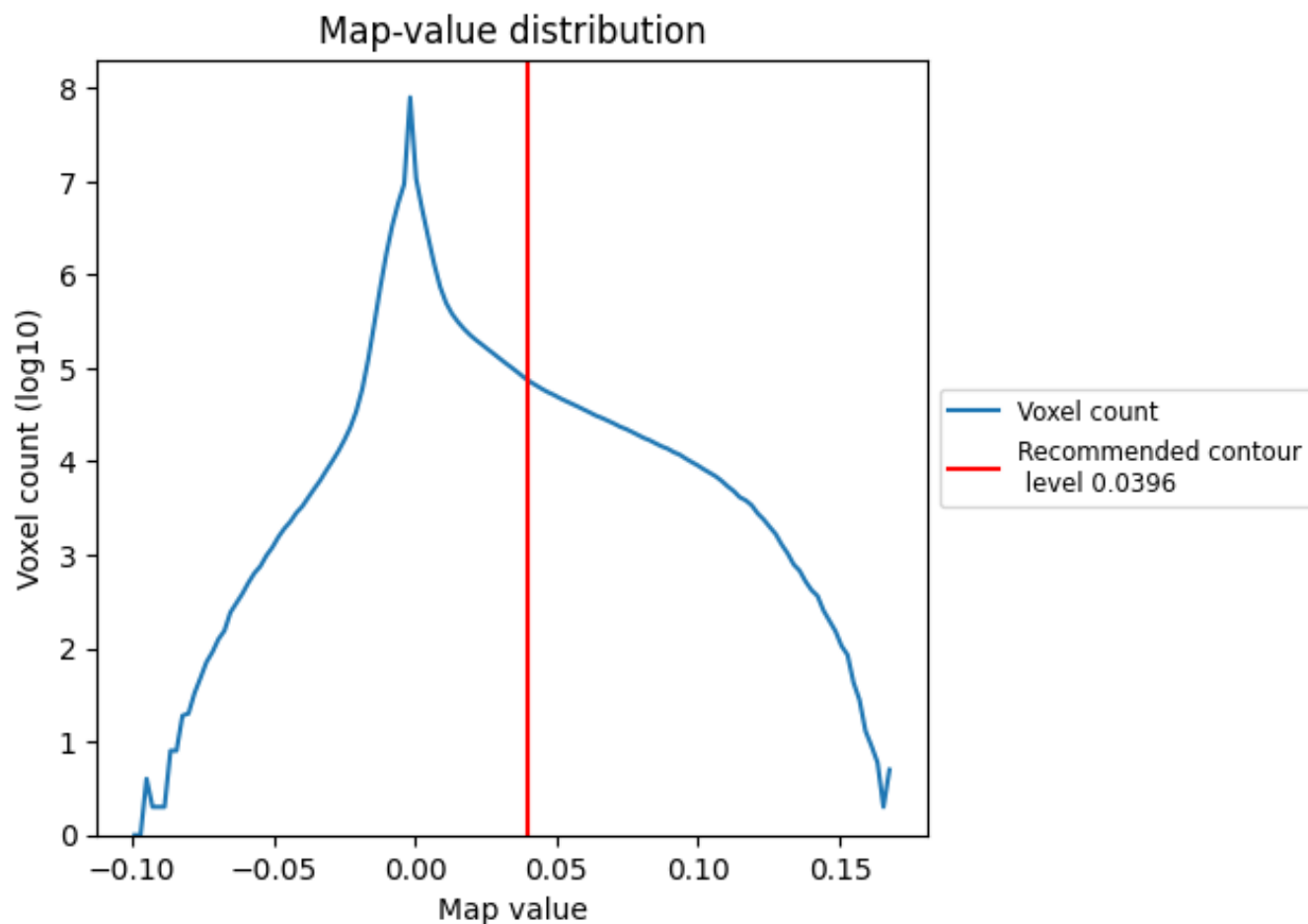
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

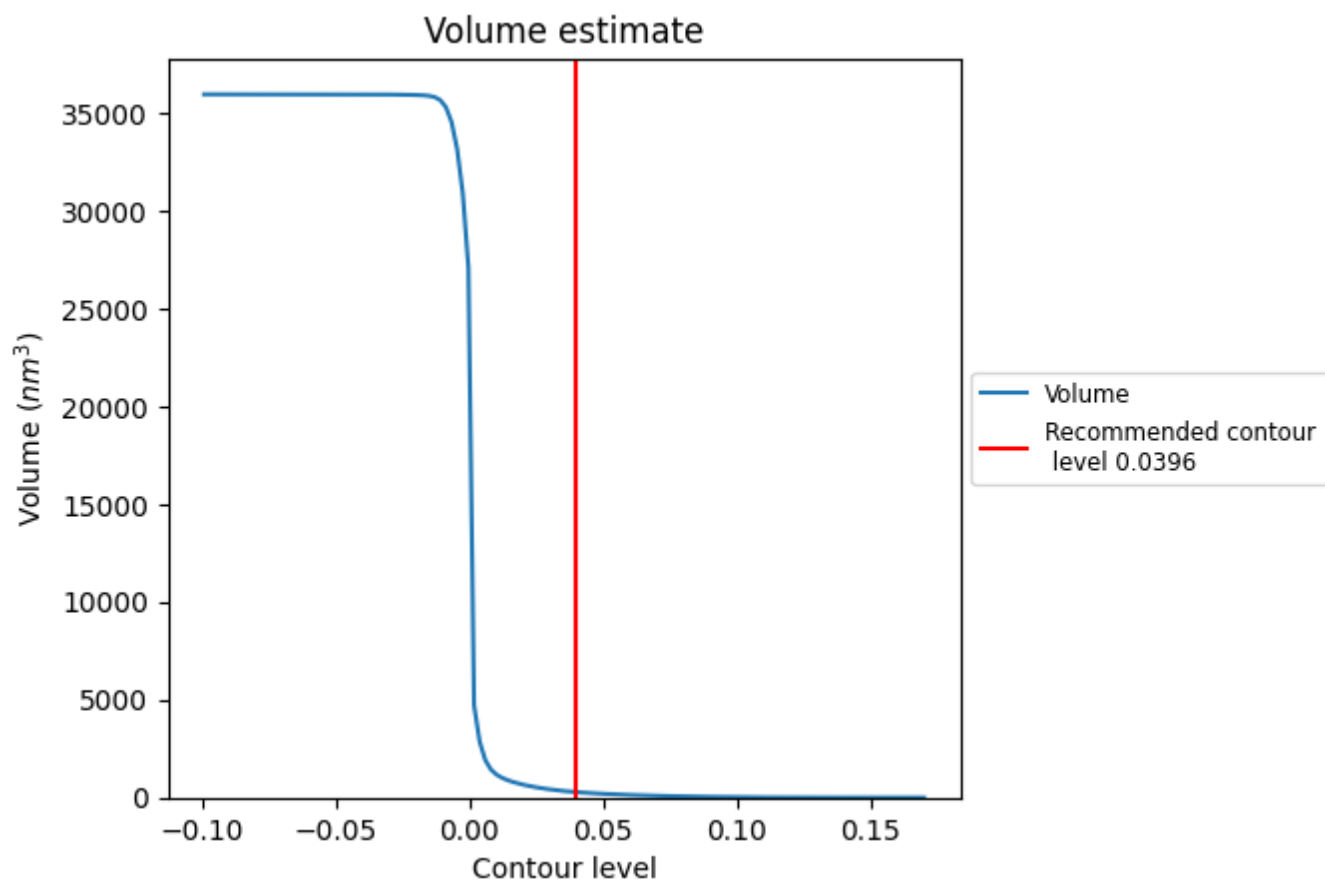
This section contains the results of statistical analysis of the map.

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.

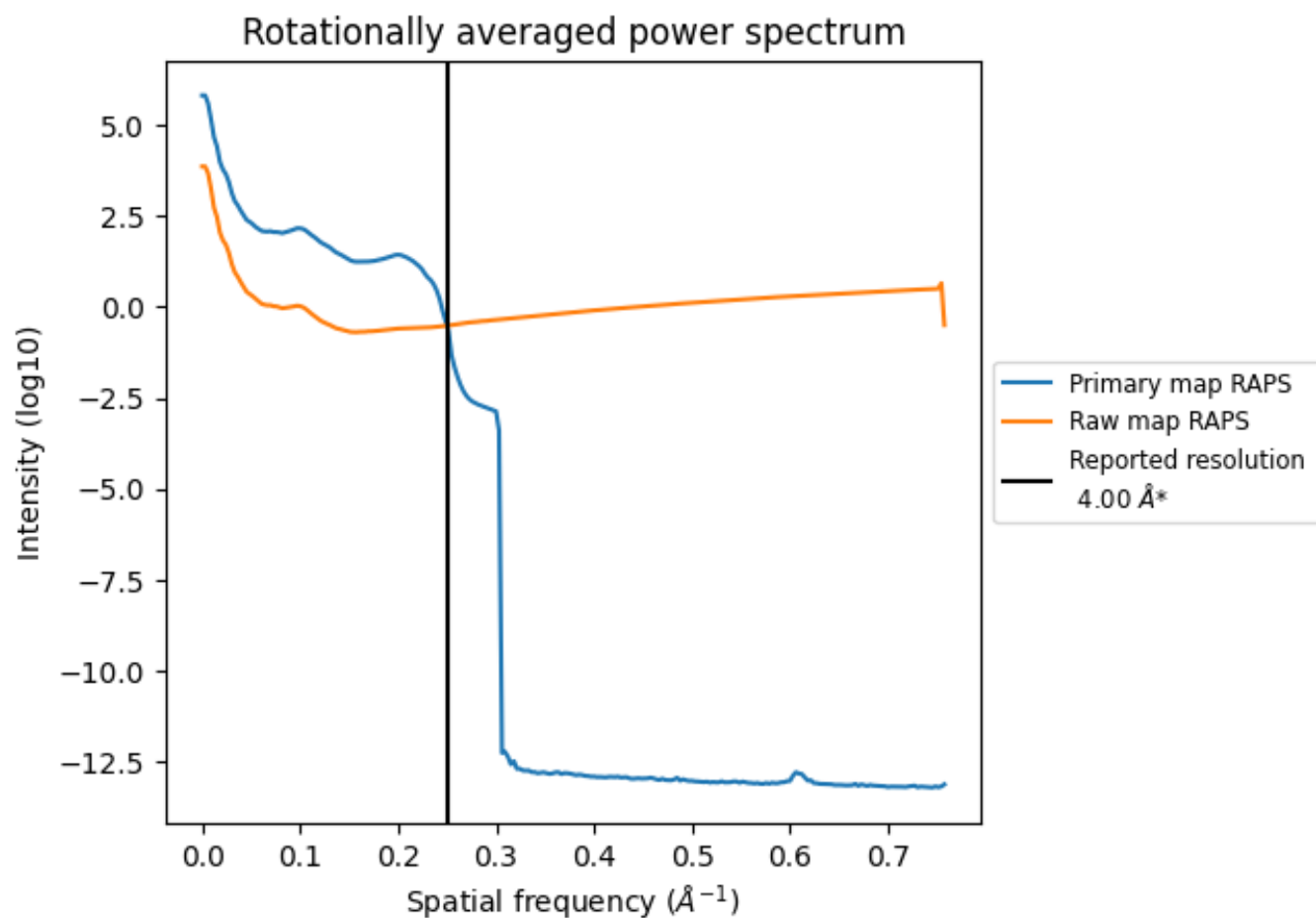
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 255 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 ⓘ

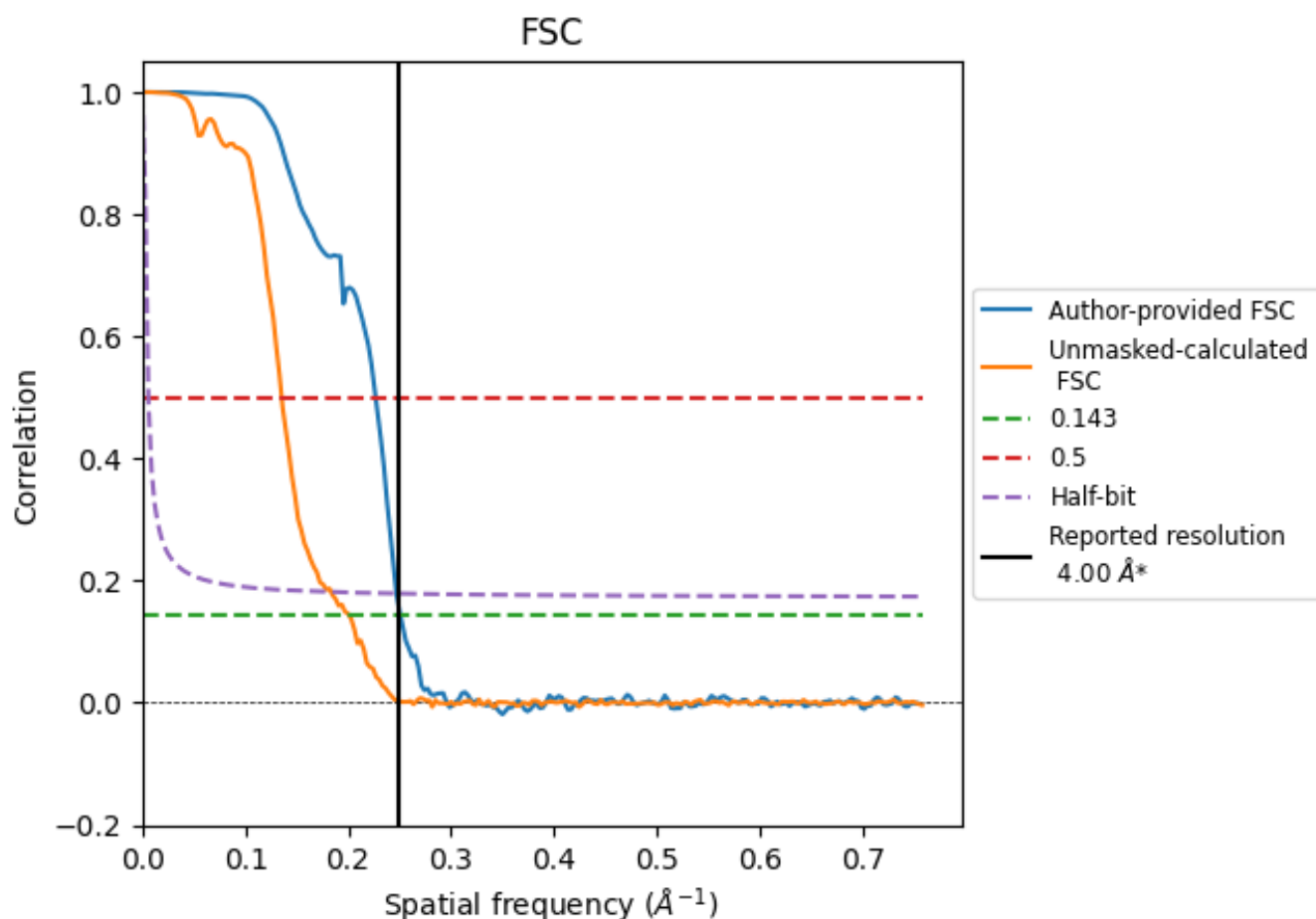


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	4.41	4.05
Unmasked-calculated*	4.98	7.39	5.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.98 differs from the reported value 4.0 by more than 10 %

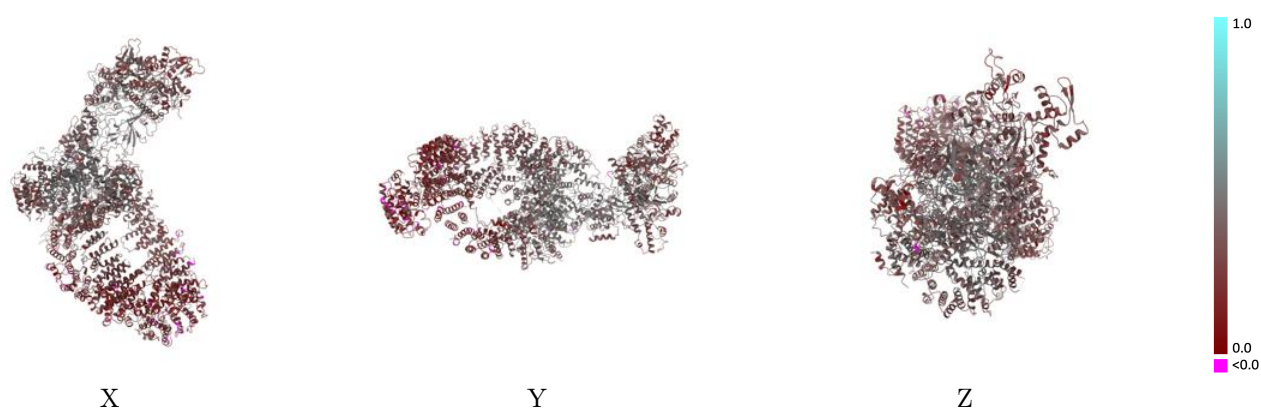
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-33796 and PDB model 7YFP. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

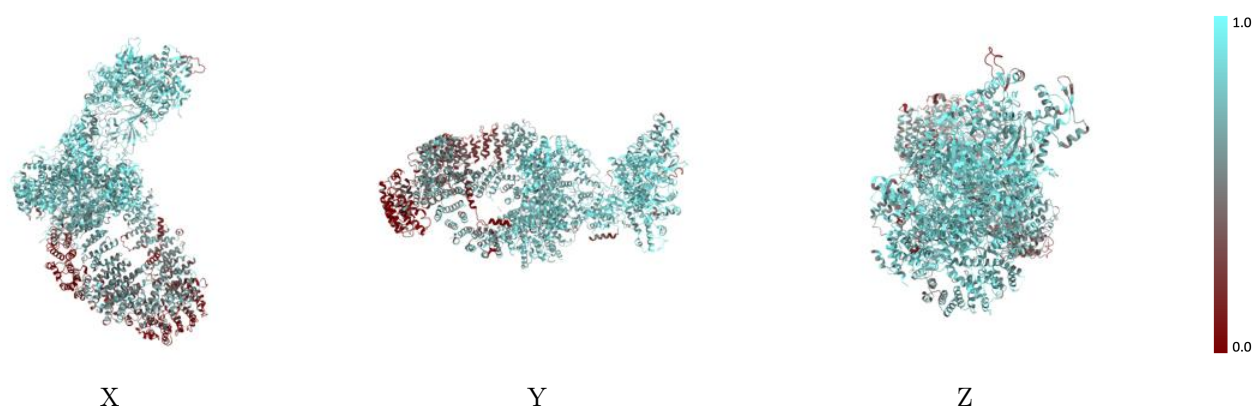
This section was not generated.

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



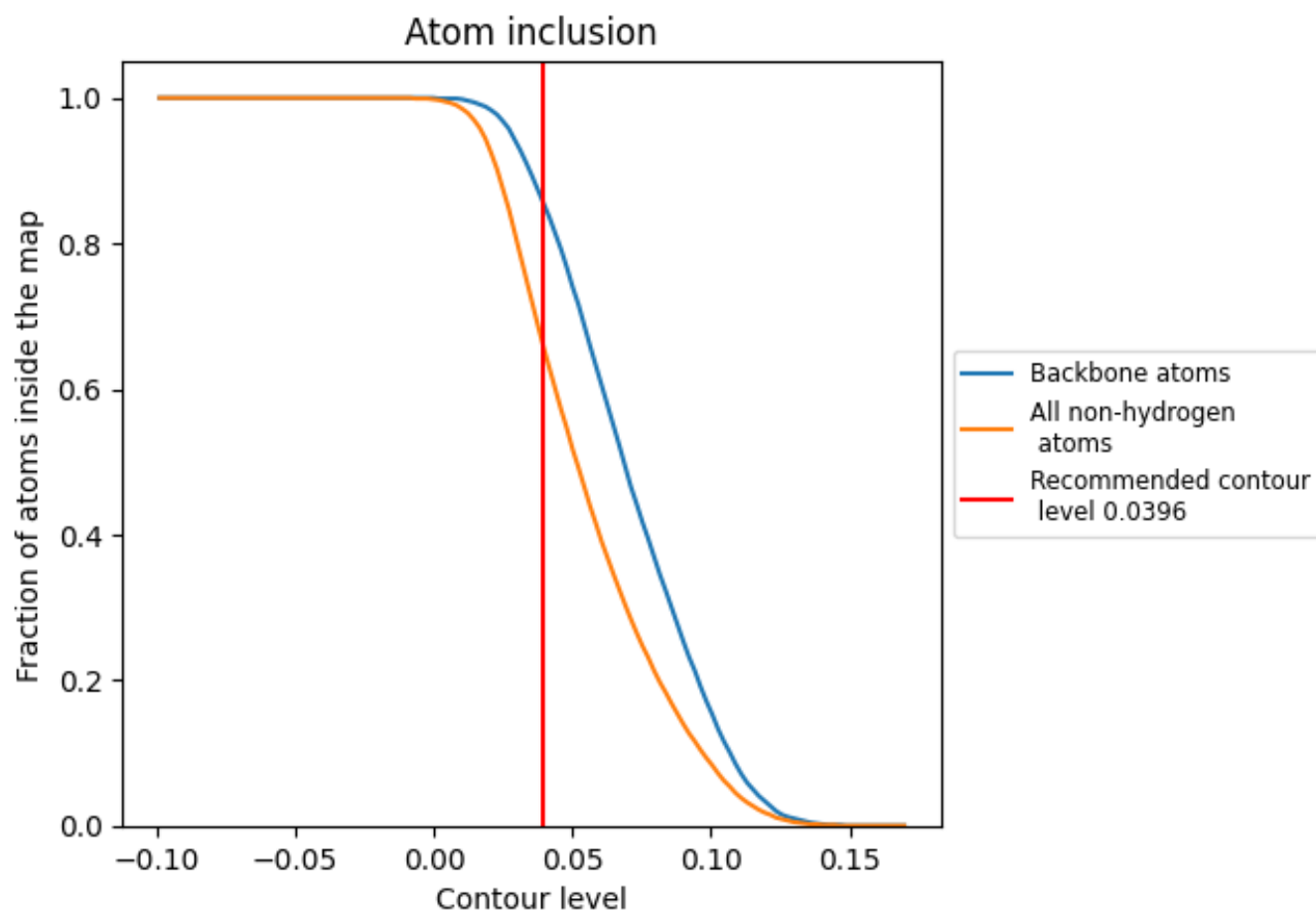
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0396).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 66% 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 (0.0396) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3340
A	0.7470	0.3330
B	0.8340	0.3930
D	0.7720	0.3870
E	0.7870	0.3540
F	0.7500	0.4060
T	0.6020	0.3170

