



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:10 AM UTC

PDB ID : 5YUD / pdb_00005yud
EMDB ID : EMD-6845
Title : Flagellin derivative in complex with the NLR protein NAIP5
Authors : Yang, X.R.; Yang, F.; Wang, W.G.; Lin, G.Z.
Deposited on : 2017-11-21
Resolution : 4.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

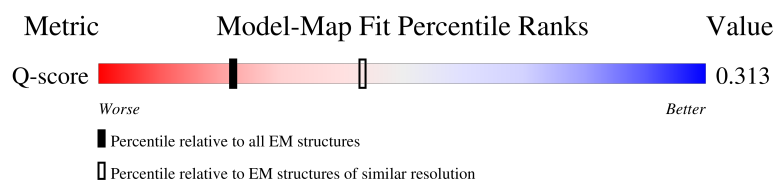
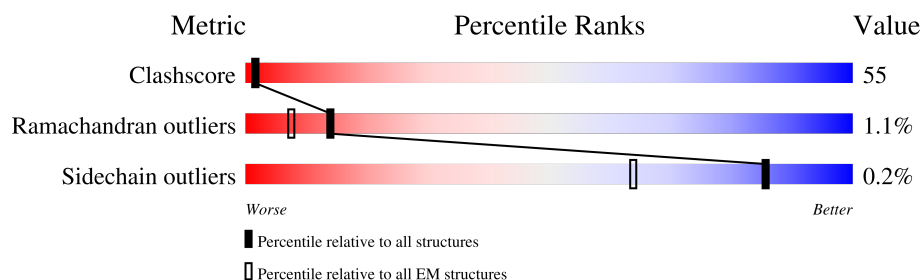
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.28 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	4493 (3.79 - 4.78)

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	1403	
2	C	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	1501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10510 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 Baculoviral IAP repeat-containing protein 1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1238	9943	6364	1671	1855	53	0	0

- Molecule 2 is a protein called Phase 2 flagellin,Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	75	536	317	103	115	1	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	421	ALA	-	expression tag	UNP P52616
C	422	ALA	-	expression tag	UNP P52616
C	423	ALA	-	expression tag	UNP P52616
C	446	SER	-	linker	UNP P52616
C	447	GLY	-	linker	UNP P52616
C	448	SER	-	linker	UNP P52616
C	449	GLY	-	linker	UNP P52616
C	450	SER	-	linker	UNP P52616
C	451	GLY	-	linker	UNP P52616

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

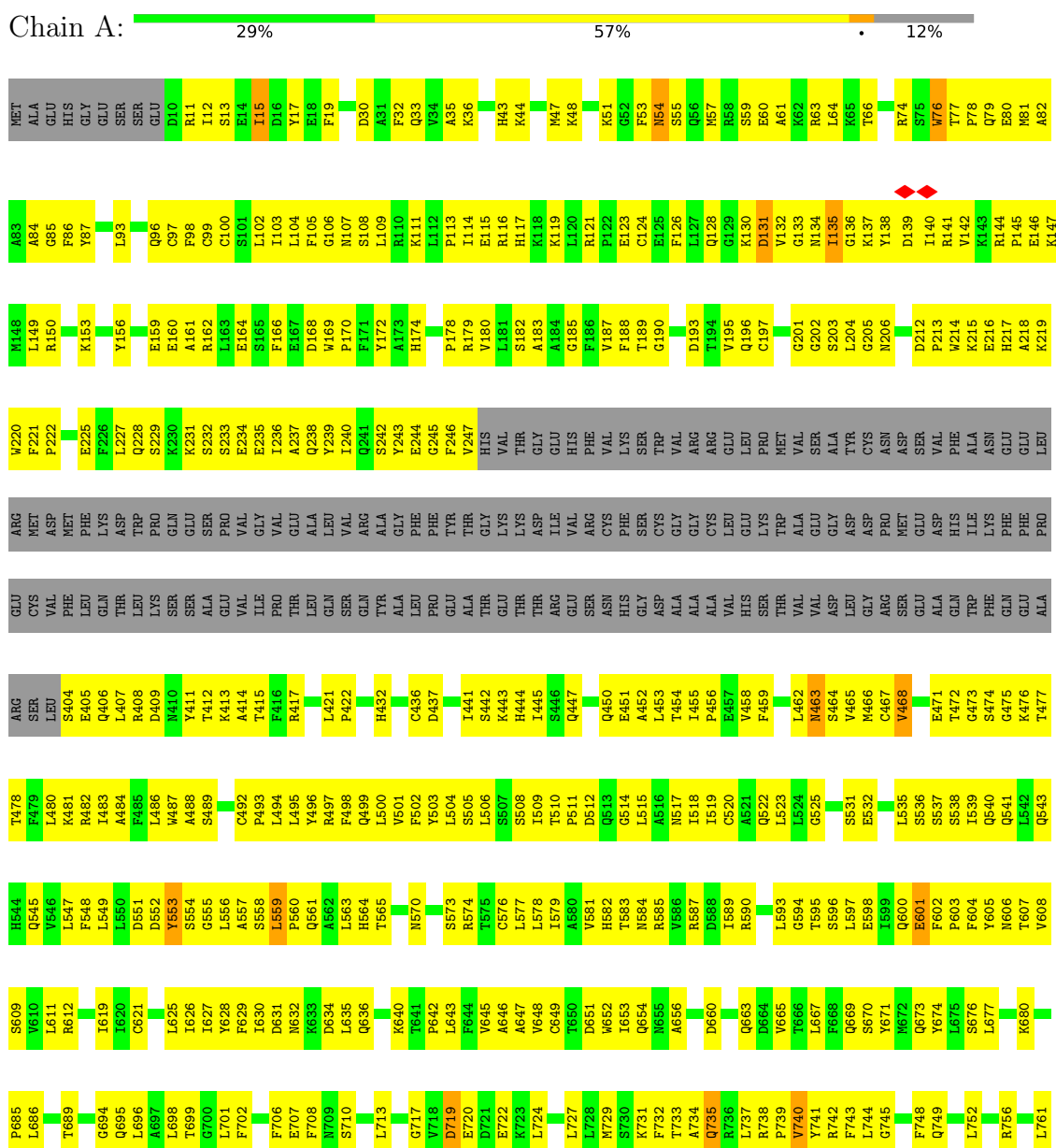


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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: Baculoviral IAP repeat-containing protein 1e



D1367	H1303	L1240	S1172	K1105	C1045	L982	L917	L840	S762
E1368	K1304	L1241	L1173	E1106	P1046	P983	K918	W841	S763
E1369	I1305	V1242	M1174	L1107	A1047	D984	V919	F842	S764
D1370	T1306	P1243	C1108	C1109	L1048	I985	S920	W849	Q766
M1371	E1307	T1244	A1175	E1049	E1049	S986	I921	W849	Q765
K1372	E1308	G1245	L1177	R1110	L1050	E987	N922	L850	Q767
V1373	G1309	D1246		L1111	S1051	G988		V851	D768
M1375	Y1310	G1247	L1183		K1052	Y989	K925	S852	Q769
K1378	R1311	L1248	E1184	K1114	A1053	W990	K926	S855	L770
E1379	N1312	H1249	E1185		S1054	K991	S927	L771	Q770
R1380	F1313	Q1250	I1186	V1117	V1055	L992	V930	S856	G772
H1381	F1314	V1251	E1187	L1118	T1056	S993		S857	L773
K1382	Q1315	A1252	F1188	S1119	K1057	P994	S933	S858	V774
P1383	A1316	K1253	S1189	V1120	C1058	K995	P934	F859	V775
Q1384	L1317	L1254	G1190	L1121	S1059	P996	K935	V860	L776
		L1255		P1122	M1060	C997	T936	R777	Q777
L1320	L1320	V1256	F1193	R1123	S1061	K998	Y937	R366	I779
P1321	P1321	E1194	A1195	F1125	R1062	I999	F938		D780
L1323	L1323	R1257		P1126	E1064	P1000	E939	A872	S781
Q1324	Q1324		F1198		L1065	L1002	N940	E873	F782
W1391	E1325	L1261	V1199	M1131	S1066	E1003	L941	I874	L783
K1392	L1326	P1262	N1200	E1132	A1068		Q942	K874	A785
L1393	N1327	C1264	T1201	K1133	E1069	N1007	P944	I786	I786
I1394	T1328	L1265	L1265	L1134	Q1070	N1008	A945	N787	N787
V1395	C1329	R1266	P1203	S1135	E1071	I1009	I946	S882	S788
R1330	R1330	V1267	N1204	I1136	E1071	D1010	T948	P883	F789
P1396				Q1137	L1072	A1011	E948	F884	N790
F1397	N1331	L1268	S1207	T1138	L1073	A1012		I885	Y795
S1398	I1332	T1269	T1269	E1141	T1074		S951	Q887	
P1399	F1333	F1270	K1208	S1142	P1076	A1015	S952	F888	S798
V1400	G1334	H1271	L1208	L1143	L1077	L1016	A953	L889	H799
	R1335	D1272	L1210	L1144	A1078	L1017	F954	R890	
L1336	I1336	L1273	L1211	S1145	L1079	Q1018	E955	K891	
Q1337	L1338	D1275	L1213	K1145	Q1080	V1019	H956	T892	K803
L1340	Q1339	D1276	K1214	K1146	S1081	L1020	T933	K993	A804
T1341	L1340	D1277	D1215	L1147	L1082	I957	L894	S958	
T1342	T1341	S1278	Q1216	V1148	E1083	S958	E959	L895	S810
V1343	L1342	V1279	Q1217	K1149	V1084	W960	L896	L896	H811
	V1343	L1280	F1218	F1150	E1086	R961	R962	V898	L812
	E1281	E1281	P1219	I1151	S1085	F1024	N963	L899	Q814
L1346	L1346	L1282	E1222	Q1152	T1087		Q866	L815	
V1350	V1350	A1283	T1223	N1153	N1088	S1027	D967	N900	L822
S1351	S1351	A1285	S1224	F1154	Q1089	I970	F904	S825	
R1352	A1286	E1225	E1225		L1090	S1029	R905	S826	M825
L1353	T1287	K1226	K1226	L1157	P1091	E1031	K972	D906	E827
P1354		F1227	V1159	H1158	E1092	I1030	N974	H907	N828
S1355	F1291	A1228	F1160	V1159	Q1093	F1032	Y974	P908	
L1356	Q1292	Q1229	H1161	L1161	L1094	R1033	E975	E909	M832
L1357	K1293	A1230	L1162	L1162	F1095	L1034	R976		K833
R1358	L1294	L1231	K1163	K1163	H1096	F1035	N976	L834	H835
L1359	E1295	G1232	C1164	C1164	N1097	N1036	Y374	L914	
H1360	N1296	S1233	D1165	D1165	L1098	S1037	E975	R915	T838
M1361	L1297	L1234	F1166	F1166	H1099	S1038	R976	S916	F839
L1362	D1298	L1235	L1167	L1167	K1100	G1039	I977	L912	
S1363	L1299	N1236	S1168	S1168	F1101	F1040	R978	L834	L834
W1364	S1300	L1237	N1169	N1169	L1041	L1041	P979	L913	H835
L1365	M1301	E1238	C1170	C1170	G1102	E1042	R980	L914	
L1366	N1302	E1239	E1239	E1171	L1104	S1043	A961	R915	T838

● Molecule 2: Phase 2 flagellin,Flagellin

Chain C:  56% 44%

A421	S427	K435	G440	Q441	A442	I443	S450	G451	S452	R453	I454	E455	D456	S457	D458	Y459	A460	T461	E462	V463	S464	N465	M466	S467	Q470	I471	L472	T477	V478	V479	L480	A481	Q482	A483	V486	P487	Q488	L491	R495
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	626608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.233	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0252	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	1/10157 (0.0%)	0.77	20/13734 (0.1%)
2	C	0.36	0/537	0.63	0/723
All	All	0.40	1/10694 (0.0%)	0.77	20/14457 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	TRP	C-N	-6.80	1.19	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	907	HIS	CA-C-N	-20.58	94.12	119.84
1	A	907	HIS	C-N-CA	-20.58	94.12	119.84
1	A	903	TYR	N-CA-C	-18.57	90.76	113.41
1	A	1273	ILE	N-CA-C	7.74	125.43	109.34
1	A	54	ASN	N-CA-C	7.53	119.76	108.31
1	A	131	ASP	N-CA-C	7.23	120.22	111.40
1	A	1373	VAL	CA-C-N	-7.17	113.97	122.22
1	A	1373	VAL	C-N-CA	-7.17	113.97	122.22
1	A	947	ASP	N-CA-C	7.04	125.79	110.80
1	A	909	GLU	N-CA-C	-6.75	99.43	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1245	GLY	N-CA-C	6.62	119.54	111.93
1	A	1066	SER	CB-CA-C	-6.35	108.59	117.23
1	A	1170	CYS	CB-CA-C	-6.35	109.24	116.54
1	A	54	ASN	CB-CA-C	-6.28	109.32	116.54
1	A	1383	GLN	N-CA-C	6.04	118.60	109.41
1	A	719	ASP	CB-CA-C	-6.03	109.64	116.63
1	A	1351	SER	CB-CA-C	-5.96	109.13	117.23
1	A	559	LEU	CA-C-N	-5.87	112.51	119.84
1	A	559	LEU	C-N-CA	-5.87	112.51	119.84
1	A	1382	PRO	N-CA-C	5.80	119.62	111.33

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1141	GLU	Peptide
1	A	1219	PRO	Peptide
1	A	1236	ASN	Peptide
1	A	1331	ASN	Peptide
1	A	1381	HIS	Peptide
1	A	652	TRP	Peptide
1	A	735	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9943	0	9933	1134	0
2	C	536	0	530	54	0
3	A	31	0	12	9	0
All	All	10510	0	10475	1163	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 55.

All (1163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG12	1:A:492:CYS:SG	1.40	1.60
1:A:135:ILE:CG2	1:A:492:CYS:HA	1.27	1.57
1:A:1274:LEU:HD21	1:A:1299:ILE:CD1	1.09	1.51
1:A:1274:LEU:CD2	1:A:1299:ILE:HD13	1.04	1.51
1:A:635:LEU:CD1	1:A:636:GLN:HG3	1.42	1.46
1:A:135:ILE:HG23	1:A:492:CYS:CA	1.56	1.35
1:A:509:ILE:CD1	1:A:518:ILE:HG23	1.56	1.33
1:A:509:ILE:HD13	1:A:518:ILE:CG2	1.58	1.33
1:A:135:ILE:CG1	1:A:492:CYS:SG	2.17	1.31
1:A:635:LEU:HD12	1:A:636:GLN:N	1.43	1.31
1:A:59:SER:OG	1:A:132:VAL:HG13	1.30	1.29
1:A:59:SER:OG	1:A:132:VAL:CG1	1.80	1.29
1:A:59:SER:CB	1:A:132:VAL:HG13	1.61	1.28
1:A:131:ASP:OD2	1:A:132:VAL:HG23	1.28	1.26
1:A:98:PHE:HE2	1:A:131:ASP:OD2	1.15	1.25
1:A:553:TYR:HE2	1:A:585:ARG:NE	1.33	1.24
1:A:553:TYR:HD2	1:A:585:ARG:CG	1.50	1.24
1:A:1321:PRO:HB3	1:A:1351:SER:OG	1.31	1.23
1:A:635:LEU:HD11	1:A:636:GLN:CG	1.69	1.23
1:A:553:TYR:CE2	1:A:585:ARG:NE	2.10	1.20
1:A:409:ASP:OD1	1:A:500:LEU:HD21	1.40	1.19
1:A:635:LEU:CD1	1:A:636:GLN:CG	2.21	1.19
1:A:1274:LEU:CD2	1:A:1299:ILE:CD1	1.82	1.19
1:A:553:TYR:CD2	1:A:585:ARG:HG3	1.76	1.18
1:A:98:PHE:CE2	1:A:131:ASP:OD2	1.95	1.17
1:A:1135:SER:O	1:A:1136:ILE:HG13	1.39	1.17
1:A:628:TYR:O	1:A:635:LEU:HD22	1.46	1.12
1:A:137:LYS:CE	1:A:140:ILE:HD12	1.78	1.12
1:A:76:TRP:CH2	1:A:116:ARG:HD3	1.85	1.12
1:A:1321:PRO:CB	1:A:1351:SER:OG	1.98	1.11
1:A:11:ARG:HD2	1:A:53:PHE:CB	1.81	1.10
1:A:553:TYR:CD2	1:A:585:ARG:CG	2.32	1.09
1:A:76:TRP:HH2	1:A:116:ARG:HD3	0.93	1.09
1:A:131:ASP:OD2	1:A:132:VAL:CG2	2.01	1.07
1:A:135:ILE:CG2	1:A:492:CYS:CA	2.22	1.07
1:A:553:TYR:CD2	1:A:585:ARG:CD	2.38	1.07
1:A:628:TYR:C	1:A:635:LEU:HD22	1.80	1.05
1:A:11:ARG:HD2	1:A:53:PHE:HB3	1.39	1.05
1:A:628:TYR:O	1:A:635:LEU:CD2	2.04	1.04
1:A:17:TYR:CE1	1:A:102:LEU:HD12	1.94	1.03
1:A:947:ASP:O	1:A:950:TYR:N	1.93	1.02
1:A:135:ILE:HG21	1:A:492:CYS:HA	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:OD1	1:A:500:LEU:CD2	2.08	1.01
1:A:32:PHE:HB2	1:A:977:ILE:HG22	1.42	1.01
1:A:12:ILE:HG22	1:A:13:SER:H	1.26	1.00
1:A:1359:LEU:HD13	1:A:1388:ILE:HD11	1.43	0.99
1:A:1274:LEU:HD11	1:A:1299:ILE:HG21	1.43	0.99
1:A:135:ILE:CD1	1:A:492:CYS:SG	2.51	0.98
1:A:635:LEU:HD12	1:A:636:GLN:CA	1.93	0.97
1:A:873:TYR:CZ	1:A:903:TYR:HB3	1.99	0.97
1:A:740:VAL:HG12	1:A:741:TYR:H	1.31	0.95
1:A:560:PRO:HA	1:A:564:HIS:HB3	1.48	0.95
1:A:137:LYS:NZ	1:A:140:ILE:HD12	1.81	0.95
1:A:635:LEU:CD1	1:A:636:GLN:N	2.31	0.94
1:A:553:TYR:HE2	1:A:585:ARG:HE	1.00	0.94
1:A:100:CYS:HG	1:A:117:HIS:HE2	1.09	0.93
1:A:947:ASP:O	1:A:949:GLU:N	2.02	0.93
1:A:1331:ASN:HB3	1:A:1334:GLY:H	1.32	0.93
1:A:60:GLU:H	1:A:132:VAL:HG11	1.34	0.93
1:A:947:ASP:OD2	1:A:1336:ILE:HD13	1.69	0.93
1:A:553:TYR:CD2	1:A:585:ARG:HD2	2.03	0.92
1:A:76:TRP:HH2	1:A:116:ARG:CD	1.82	0.92
1:A:628:TYR:CA	1:A:635:LEU:HD22	1.99	0.92
1:A:1170:CYS:SG	1:A:1171:GLU:N	2.41	0.92
1:A:104:LEU:HD22	1:A:116:ARG:HH21	1.36	0.91
1:A:510:THR:HB	1:A:557:ALA:HB2	1.52	0.91
1:A:12:ILE:HG22	1:A:13:SER:N	1.84	0.91
1:A:984:ASP:HA	1:A:987:GLU:HB2	1.52	0.91
1:A:1274:LEU:HD22	1:A:1299:ILE:CD1	1.96	0.91
1:A:137:LYS:NZ	1:A:140:ILE:CD1	2.33	0.90
1:A:553:TYR:CE2	1:A:585:ARG:CD	2.53	0.90
1:A:135:ILE:HG22	1:A:135:ILE:O	1.71	0.89
1:A:1280:ILE:HG22	1:A:1284:ARG:HG3	1.52	0.89
1:A:131:ASP:CG	1:A:132:VAL:HG23	1.98	0.89
1:A:900:ASN:HB2	1:A:987:GLU:HA	1.55	0.88
1:A:1187:GLU:HA	1:A:1212:ASN:HB2	1.56	0.88
1:A:32:PHE:CB	1:A:977:ILE:HG22	2.02	0.88
1:A:137:LYS:HZ1	1:A:140:ILE:CD1	1.87	0.87
1:A:635:LEU:HD11	1:A:636:GLN:HG3	0.89	0.87
1:A:33:GLN:HE21	1:A:35:ALA:H	1.16	0.87
1:A:975:GLU:HA	1:A:978:ARG:HH21	1.39	0.87
1:A:635:LEU:HD12	1:A:636:GLN:HG3	1.44	0.87
1:A:907:HIS:HB2	1:A:908:PRO:HD3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:LEU:CD2	1:A:1299:ILE:HD11	2.03	0.87
1:A:12:ILE:CG2	1:A:13:SER:H	1.88	0.87
1:A:1375:ASN:HD21	1:A:1383:GLN:CG	1.88	0.87
1:A:11:ARG:HD2	1:A:53:PHE:HB2	1.53	0.86
1:A:1248:ILE:HB	1:A:1273:ILE:HD11	1.55	0.86
1:A:1169:ASN:HD22	1:A:1193:PHE:HA	1.41	0.86
1:A:137:LYS:HE3	1:A:140:ILE:HD12	1.57	0.86
1:A:948:GLU:OE1	1:A:948:GLU:N	2.08	0.86
1:A:137:LYS:HG2	1:A:493:PRO:HB3	1.58	0.86
1:A:441:ILE:CD1	1:A:600:GLN:HB2	2.05	0.85
1:A:593:LEU:HD23	1:A:594:GLY:O	1.76	0.85
1:A:740:VAL:HG12	1:A:741:TYR:N	1.87	0.85
1:A:104:LEU:HD22	1:A:116:ARG:NH2	1.92	0.85
1:A:553:TYR:HD2	1:A:585:ARG:CD	1.85	0.85
1:A:467:CYS:HA	1:A:593:LEU:HD11	1.60	0.84
1:A:553:TYR:HD2	1:A:585:ARG:HG3	1.16	0.84
1:A:602:PHE:CE2	1:A:607:THR:HG23	2.12	0.84
1:A:1388:ILE:HG22	1:A:1389:ILE:N	1.91	0.84
1:A:17:TYR:CE1	1:A:102:LEU:CD1	2.60	0.84
1:A:1030:ILE:HB	1:A:1054:SER:HA	1.58	0.84
1:A:635:LEU:HD12	1:A:636:GLN:H	1.38	0.83
1:A:57:MET:HB2	1:A:63:ARG:HH22	1.41	0.83
1:A:464:SER:O	1:A:576:CYS:HA	1.77	0.83
1:A:740:VAL:CG1	1:A:741:TYR:H	1.91	0.83
1:A:1216:GLN:N	1:A:1244:THR:OG1	2.10	0.83
1:A:779:ILE:O	1:A:779:ILE:HG22	1.77	0.83
1:A:245:GLY:CA	1:A:463:ASN:HD21	1.92	0.82
1:A:1343:VAL:HA	1:A:1346:LEU:HG	1.60	0.82
1:A:459:PHE:HB3	1:A:494:LEU:HB2	1.61	0.81
1:A:59:SER:OG	1:A:132:VAL:HG12	1.80	0.81
1:A:510:THR:HB	1:A:557:ALA:CB	2.11	0.81
1:A:473:GLY:N	3:A:1501:ATP:O2G	2.12	0.81
1:A:947:ASP:HB2	1:A:950:TYR:HB2	1.63	0.81
1:A:632:ASN:O	1:A:635:LEU:HG	1.81	0.80
1:A:1375:ASN:HD21	1:A:1383:GLN:HG2	1.45	0.80
1:A:422:PRO:HB3	1:A:432:HIS:HB3	1.62	0.80
1:A:245:GLY:HA3	1:A:463:ASN:HD21	1.46	0.80
1:A:986:SER:O	1:A:990:TRP:N	2.14	0.80
1:A:1350:VAL:O	1:A:1351:SER:OG	2.00	0.80
1:A:467:CYS:HB2	1:A:597:LEU:H	1.44	0.79
1:A:61:ALA:HB2	1:A:134:ASN:OD1	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LEU:HD12	1:A:636:GLN:CG	2.02	0.79
1:A:873:TYR:CE2	1:A:903:TYR:HB3	2.17	0.79
1:A:1301:MET:O	1:A:1305:ILE:HD11	1.83	0.79
1:A:1327:ASN:ND2	2:C:462:GLU:OE2	2.14	0.79
1:A:628:TYR:HA	1:A:635:LEU:HD22	1.64	0.79
1:A:1055:VAL:HA	1:A:1079:LEU:HA	1.63	0.79
1:A:1213:LEU:H	1:A:1241:LEU:HB2	1.47	0.79
1:A:553:TYR:O	1:A:554:SER:OG	2.00	0.79
1:A:1388:ILE:HG23	2:C:465:ASN:CG	2.08	0.78
1:A:893:THR:HG22	1:A:914:LEU:HB2	1.64	0.78
1:A:634:ASP:OD1	1:A:835:HIS:ND1	2.16	0.78
1:A:902:GLN:O	1:A:990:TRP:NE1	2.15	0.78
1:A:946:ILE:HG22	1:A:947:ASP:H	1.46	0.78
1:A:556:LEU:HD12	1:A:556:LEU:O	1.84	0.78
1:A:589:ILE:O	1:A:589:ILE:HG12	1.81	0.78
1:A:1173:LEU:O	1:A:1177:LEU:N	2.14	0.78
1:A:989:TYR:O	1:A:993:SER:N	2.16	0.78
1:A:59:SER:CB	1:A:132:VAL:CG1	2.48	0.77
1:A:1388:ILE:HG23	2:C:465:ASN:OD1	1.84	0.77
1:A:1066:SER:OG	1:A:1067:ARG:N	2.16	0.77
1:A:1135:SER:O	1:A:1136:ILE:CG1	2.28	0.77
1:A:1324:GLN:HA	1:A:1354:PRO:HD2	1.65	0.77
1:A:1301:MET:O	1:A:1305:ILE:CD1	2.32	0.77
1:A:1394:ILE:HG23	1:A:1396:PRO:HD3	1.65	0.77
1:A:441:ILE:HD11	1:A:600:GLN:HB2	1.67	0.77
1:A:548:PHE:HB2	1:A:577:LEU:HG	1.66	0.77
2:C:461:THR:HG22	2:C:465:ASN:HD21	1.49	0.77
1:A:59:SER:CA	1:A:132:VAL:HG13	2.13	0.77
1:A:1062:ARG:NH1	1:A:1086:GLU:OE1	2.18	0.77
1:A:510:THR:O	1:A:557:ALA:HB1	1.85	0.77
1:A:468:VAL:H	1:A:597:LEU:HB2	1.48	0.76
1:A:135:ILE:HG12	1:A:492:CYS:HG	1.47	0.76
1:A:1216:GLN:H	1:A:1244:THR:HG1	1.30	0.76
1:A:520:CYS:HA	1:A:523:LEU:HB2	1.68	0.76
1:A:1053:ALA:HA	1:A:1077:PRO:HB3	1.68	0.76
1:A:417:ARG:HE	1:A:488:ALA:HB1	1.48	0.76
1:A:1252:ALA:HB2	1:A:1273:ILE:HD13	1.66	0.76
1:A:1359:LEU:HD13	1:A:1388:ILE:CD1	2.15	0.76
1:A:32:PHE:HB2	1:A:977:ILE:CG2	2.15	0.76
1:A:1274:LEU:HD21	1:A:1299:ILE:CG1	2.11	0.75
1:A:135:ILE:HG23	1:A:492:CYS:HA	0.76	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LYS:H	1:A:596:SER:HB2	1.51	0.75
1:A:1274:LEU:CG	1:A:1299:ILE:HD13	2.12	0.75
1:A:719:ASP:CG	1:A:720:GLU:H	1.93	0.75
1:A:59:SER:HA	1:A:132:VAL:CG1	2.17	0.75
1:A:604:PHE:O	1:A:607:THR:OG1	2.04	0.75
1:A:135:ILE:HG23	1:A:492:CYS:C	2.12	0.74
1:A:137:LYS:HD3	1:A:493:PRO:HA	1.69	0.74
1:A:902:GLN:HB3	1:A:905:ARG:N	2.02	0.74
1:A:59:SER:CA	1:A:132:VAL:CG1	2.65	0.74
1:A:1007:ASN:O	1:A:1037:SER:N	2.14	0.74
1:A:800:SER:HB2	1:A:874:GLU:HG3	1.67	0.74
1:A:1298:ASP:O	1:A:1299:ILE:HG13	1.87	0.74
1:A:135:ILE:HG12	1:A:492:CYS:CB	2.17	0.74
1:A:873:TYR:CE1	1:A:903:TYR:HD2	2.06	0.74
1:A:80:GLU:HB3	1:A:113:PRO:HG3	1.70	0.74
1:A:44:LYS:HG2	1:A:105:PHE:HD2	1.53	0.73
1:A:1365:LEU:O	1:A:1369:GLU:N	2.21	0.73
1:A:1055:VAL:HG12	1:A:1056:THR:H	1.52	0.73
1:A:999:ILE:HB	1:A:1027:SER:HA	1.68	0.73
1:A:1030:ILE:O	1:A:1056:THR:OG1	2.05	0.73
1:A:531:SER:O	1:A:535:LEU:N	2.21	0.73
1:A:132:VAL:HG12	1:A:133:GLY:N	2.02	0.73
1:A:135:ILE:HD11	1:A:492:CYS:SG	2.28	0.73
1:A:587:ARG:NH1	1:A:733:THR:O	2.22	0.73
1:A:504:LEU:HD13	1:A:518:ILE:HG22	1.70	0.72
1:A:1307:GLU:O	1:A:1339:GLN:NE2	2.22	0.72
1:A:1280:ILE:CG2	1:A:1284:ARG:HG3	2.19	0.72
1:A:1364:TRP:O	1:A:1368:GLU:N	2.21	0.72
1:A:137:LYS:CE	1:A:140:ILE:CD1	2.65	0.72
1:A:1133:LYS:HE2	1:A:1161:HIS:HD2	1.52	0.72
1:A:1050:LEU:HB2	1:A:1052:LYS:HZ2	1.54	0.72
1:A:535:LEU:O	1:A:539:ILE:N	2.18	0.72
1:A:1309:GLY:O	1:A:1313:PHE:N	2.19	0.72
1:A:1375:ASN:ND2	1:A:1383:GLN:HG2	2.05	0.72
1:A:480:LEU:HB3	1:A:549:LEU:HD23	1.71	0.72
1:A:947:ASP:O	1:A:948:GLU:C	2.31	0.72
1:A:476:LYS:NZ	1:A:582:HIS:HA	2.05	0.71
1:A:948:GLU:H	1:A:948:GLU:CD	1.97	0.71
1:A:138:TYR:HE1	1:A:206:ASN:HB2	1.54	0.71
1:A:873:TYR:CE1	1:A:903:TYR:CD2	2.78	0.71
1:A:1251:VAL:HA	1:A:1253:LYS:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:CYS:O	3:A:1501:ATP:N6	2.24	0.71
1:A:1012:ALA:HA	1:A:1017:LEU:HD11	1.71	0.71
1:A:1252:ALA:CB	1:A:1273:ILE:HD13	2.21	0.71
1:A:77:THR:HB	1:A:80:GLU:HG3	1.73	0.70
1:A:482:ARG:HG2	1:A:486:LEU:CD1	2.21	0.70
1:A:763:SER:HB2	1:A:803:LYS:HD2	1.71	0.70
1:A:1253:LYS:O	1:A:1257:ARG:N	2.21	0.70
2:C:479:VAL:O	2:C:483:ALA:N	2.24	0.70
1:A:1089:GLN:HE21	1:A:1094:LEU:HB3	1.55	0.70
1:A:1135:SER:C	1:A:1136:ILE:HG13	2.16	0.70
1:A:1154:PHE:HA	1:A:1157:LEU:HG	1.74	0.70
1:A:1311:ARG:HG2	1:A:1339:GLN:HE21	1.56	0.70
1:A:1358:ARG:HB2	1:A:1361:MET:HE2	1.72	0.70
1:A:1142:SER:OG	1:A:1168:SER:O	2.08	0.70
1:A:1388:ILE:CG2	1:A:1389:ILE:N	2.55	0.70
1:A:464:SER:C	1:A:576:CYS:HA	2.17	0.70
1:A:602:PHE:CE2	1:A:603:PRO:O	2.45	0.70
1:A:11:ARG:HG2	1:A:12:ILE:N	2.07	0.69
1:A:437:ASP:O	1:A:606:ASN:ND2	2.25	0.69
1:A:640:LYS:HE3	1:A:745:GLY:HA3	1.75	0.69
1:A:498:PHE:HD1	1:A:545:GLN:HA	1.57	0.69
1:A:602:PHE:CD2	1:A:603:PRO:O	2.46	0.69
1:A:501:VAL:HG22	1:A:547:LEU:HD23	1.73	0.69
1:A:60:GLU:N	1:A:132:VAL:HG11	2.05	0.69
1:A:949:GLU:CD	1:A:1365:LEU:H	2.00	0.69
1:A:1310:TYR:O	1:A:1314:PHE:N	2.25	0.69
1:A:236:ILE:O	1:A:240:ILE:N	2.26	0.69
1:A:1274:LEU:CD1	1:A:1299:ILE:HG21	2.23	0.69
2:C:453:ARG:HA	2:C:456:ASP:HB3	1.75	0.69
1:A:558:SER:HA	1:A:563:LEU:CD2	2.22	0.69
1:A:795:TYR:O	1:A:798:SER:OG	2.07	0.69
1:A:1343:VAL:HG13	1:A:1346:LEU:HD12	1.73	0.69
1:A:137:LYS:HZ1	1:A:140:ILE:HD12	1.48	0.69
1:A:537:SER:HA	1:A:540:GLN:HG2	1.75	0.69
1:A:60:GLU:O	1:A:63:ARG:N	2.24	0.68
1:A:1169:ASN:ND2	1:A:1193:PHE:HA	2.07	0.68
1:A:1040:PHE:O	1:A:1043:SER:OG	2.11	0.68
1:A:916:SER:HA	1:A:1003:GLU:HB2	1.75	0.68
1:A:135:ILE:CG2	1:A:135:ILE:O	2.42	0.68
1:A:945:ALA:HB1	1:A:1399:PRO:HG2	1.75	0.68
1:A:1088:ASN:HB3	1:A:1114:LYS:HZ2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:ILE:HA	1:A:1283:ALA:HB3	1.73	0.68
1:A:1275:ASP:H	1:A:1304:LYS:HE3	1.57	0.68
1:A:628:TYR:O	1:A:635:LEU:HD21	1.91	0.68
1:A:1314:PHE:HA	1:A:1317:LEU:HD23	1.76	0.68
1:A:570:ASN:O	1:A:574:ARG:N	2.26	0.68
1:A:654:GLN:NE2	1:A:660:ASP:OD2	2.19	0.68
1:A:665:VAL:O	1:A:669:GLN:N	2.23	0.68
1:A:984:ASP:N	1:A:987:GLU:OE1	2.26	0.68
1:A:405:GLU:HA	1:A:408:ARG:NH2	2.08	0.68
1:A:1264:CYS:HA	1:A:1293:LYS:HE2	1.76	0.68
1:A:1193:PHE:HE2	1:A:1217:GLN:HA	1.58	0.67
1:A:1252:ALA:HB2	1:A:1273:ILE:CD1	2.24	0.67
1:A:59:SER:HB2	1:A:132:VAL:HG13	1.72	0.67
1:A:441:ILE:HD12	1:A:600:GLN:HB2	1.76	0.67
1:A:482:ARG:HG2	1:A:486:LEU:HD12	1.76	0.67
1:A:956:HIS:ND1	1:A:1392:LYS:HA	2.09	0.67
1:A:988:GLY:O	1:A:992:LEU:N	2.28	0.67
1:A:197:CYS:N	1:A:202:GLY:O	2.20	0.67
1:A:939:GLU:O	1:A:943:PRO:HD3	1.94	0.67
1:A:82:ALA:O	1:A:85:GLY:N	2.23	0.67
1:A:17:TYR:HE1	1:A:102:LEU:HD12	1.54	0.67
1:A:898:VAL:HA	1:A:901:LEU:HD23	1.74	0.67
1:A:1007:ASN:HB3	1:A:1036:ASN:OD1	1.95	0.67
1:A:982:LEU:HB2	1:A:983:PRO:HD2	1.76	0.67
1:A:141:ARG:NH2	1:A:193:ASP:OD1	2.27	0.67
1:A:558:SER:HA	1:A:563:LEU:HD23	1.77	0.67
1:A:739:PRO:O	1:A:740:VAL:HG23	1.95	0.67
1:A:1008:ASN:OD1	1:A:1009:THR:N	2.27	0.66
1:A:477:THR:N	3:A:1501:ATP:O2A	2.27	0.66
1:A:552:ASP:OD1	1:A:553:TYR:N	2.24	0.66
1:A:974:TYR:CZ	1:A:978:ARG:HD3	2.30	0.66
1:A:1311:ARG:H	1:A:1339:GLN:NE2	1.94	0.66
1:A:498:PHE:HA	1:A:545:GLN:HG2	1.76	0.66
1:A:590:ARG:HH12	1:A:734:ALA:HB1	1.60	0.66
1:A:873:TYR:OH	1:A:903:TYR:HB3	1.94	0.66
1:A:1091:PRO:HA	1:A:1095:PHE:N	2.10	0.66
1:A:1184:ARG:NH2	1:A:1207:SER:OG	2.28	0.66
1:A:635:LEU:CD1	1:A:636:GLN:H	2.04	0.66
1:A:905:ARG:NH2	1:A:997:CYS:SG	2.65	0.66
1:A:918:LYS:NZ	1:A:920:SER:OG	2.24	0.66
1:A:555:GLY:O	1:A:563:LEU:HD13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:NZ	1:A:140:ILE:HD11	2.09	0.66
1:A:553:TYR:HD2	1:A:585:ARG:CB	2.08	0.65
1:A:138:TYR:HA	1:A:141:ARG:HB2	1.77	0.65
1:A:719:ASP:OD1	1:A:720:GLU:N	2.29	0.65
1:A:214:TRP:HE3	1:A:231:LYS:HD2	1.60	0.65
2:C:457:SER:O	2:C:461:THR:N	2.25	0.65
1:A:137:LYS:HZ1	1:A:140:ILE:HD11	1.60	0.65
1:A:19:PHE:HE1	1:A:108:SER:HG	1.44	0.65
1:A:701:LEU:HB3	1:A:778:GLN:HE21	1.62	0.65
1:A:1339:GLN:O	1:A:1342:THR:OG1	2.12	0.65
1:A:138:TYR:CE1	1:A:206:ASN:HB2	2.32	0.64
1:A:1160:PHE:HB3	1:A:1161:HIS:CD2	2.33	0.64
1:A:471:GLU:O	1:A:582:HIS:CD2	2.50	0.64
1:A:944:PRO:HB2	1:A:1396:PRO:HD2	1.79	0.64
1:A:543:GLN:OE1	1:A:574:ARG:NE	2.29	0.64
1:A:849:TRP:HA	1:A:856:SER:HB2	1.78	0.64
1:A:1065:LEU:HD23	1:A:1068:ALA:HB2	1.80	0.64
1:A:1210:ILE:HG12	1:A:1239:GLU:HG3	1.78	0.64
1:A:1301:MET:HE3	1:A:1302:ASN:H	1.61	0.64
1:A:587:ARG:HD3	1:A:734:ALA:HA	1.80	0.64
1:A:872:ALA:HB1	1:A:877:THR:HG22	1.80	0.64
1:A:1090:LEU:HB2	1:A:1093:GLN:HG3	1.80	0.64
1:A:1047:ALA:O	1:A:1052:LYS:NZ	2.25	0.64
1:A:1282:ILE:O	1:A:1286:ALA:N	2.31	0.64
2:C:455:GLU:HA	2:C:458:ASP:OD2	1.98	0.64
1:A:589:ILE:O	1:A:589:ILE:CG1	2.46	0.64
1:A:1254:LEU:HD23	1:A:1257:ARG:HD2	1.79	0.64
1:A:708:PHE:HB2	1:A:741:TYR:CD2	2.33	0.64
1:A:885:ILE:HG22	1:A:889:LEU:HD11	1.79	0.64
1:A:123:GLU:HG3	1:A:124:CYS:H	1.61	0.63
1:A:779:ILE:O	1:A:779:ILE:CG2	2.45	0.63
1:A:1143:ASP:OD2	1:A:1146:LYS:NZ	2.31	0.63
1:A:503:TYR:HA	1:A:549:LEU:HB2	1.81	0.63
1:A:1039:GLY:HA2	1:A:1065:LEU:HD22	1.80	0.63
1:A:1280:ILE:O	1:A:1284:ARG:N	2.28	0.63
1:A:1107:LEU:O	1:A:1135:SER:OG	2.15	0.63
1:A:713:LEU:O	1:A:717:GLY:N	2.28	0.63
1:A:132:VAL:CG1	1:A:133:GLY:N	2.61	0.63
1:A:405:GLU:HA	1:A:408:ARG:HH22	1.63	0.63
1:A:1184:ARG:NH1	1:A:1207:SER:O	2.32	0.63
1:A:1125:PHE:HZ	1:A:1149:LYS:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HG13	1:A:595:THR:HA	1.80	0.63
1:A:719:ASP:CG	1:A:720:GLU:N	2.56	0.63
1:A:1059:SER:HA	1:A:1083:GLU:HB3	1.80	0.63
1:A:676:SER:O	1:A:680:LYS:N	2.32	0.62
1:A:579:ILE:HG22	1:A:581:VAL:HG23	1.81	0.62
1:A:1060:MET:HB2	1:A:1084:VAL:HG22	1.81	0.62
1:A:1381:HIS:HB2	1:A:1382:PRO:HD3	1.80	0.62
1:A:153:LYS:HD2	1:A:156:TYR:CD2	2.34	0.62
1:A:963:ASN:O	1:A:966:GLN:HG2	1.98	0.62
1:A:473:GLY:H	3:A:1501:ATP:PG	2.21	0.62
1:A:1169:ASN:HB3	1:A:1194:GLU:HG3	1.82	0.62
1:A:1274:LEU:HB2	1:A:1304:LYS:HB3	1.82	0.62
1:A:74:ARG:HG3	1:A:93:LEU:HD21	1.81	0.62
1:A:76:TRP:CH2	1:A:116:ARG:CD	2.69	0.62
1:A:1275:ASP:N	1:A:1304:LYS:HE3	2.15	0.62
1:A:696:LEU:O	1:A:699:THR:OG1	2.15	0.62
1:A:107:ASN:O	2:C:495:ARG:NH1	2.32	0.62
1:A:213:PRO:O	1:A:217:HIS:N	2.24	0.62
1:A:986:SER:HA	1:A:989:TYR:HB2	1.82	0.62
1:A:44:LYS:HG2	1:A:105:PHE:CD2	2.34	0.61
1:A:926:MET:HE3	1:A:927:SER:H	1.64	0.61
1:A:1299:ILE:HG22	1:A:1301:MET:H	1.64	0.61
1:A:11:ARG:HG2	1:A:12:ILE:H	1.63	0.61
1:A:98:PHE:HE2	1:A:131:ASP:CG	2.02	0.61
1:A:444:HIS:CD2	1:A:447:GLN:H	2.17	0.61
1:A:1328:ILE:HG21	1:A:1335:ARG:HH22	1.64	0.61
1:A:629:PHE:O	2:C:488:GLN:NE2	2.33	0.61
1:A:1211:LEU:O	1:A:1241:LEU:N	2.33	0.61
1:A:77:THR:HG22	1:A:79:GLN:H	1.65	0.61
1:A:459:PHE:HZ	1:A:482:ARG:HH22	1.49	0.61
1:A:602:PHE:CZ	1:A:606:ASN:HB2	2.35	0.61
1:A:1346:LEU:HD13	1:A:1358:ARG:HH22	1.64	0.61
1:A:553:TYR:C	1:A:554:SER:HG	2.02	0.61
2:C:461:THR:HG22	2:C:465:ASN:ND2	2.16	0.61
1:A:1040:PHE:CE2	1:A:1044:ILE:HD11	2.35	0.61
1:A:1066:SER:HA	1:A:1093:GLN:HG2	1.81	0.61
1:A:153:LYS:HD2	1:A:156:TYR:HD2	1.66	0.60
1:A:631:ASP:HB3	1:A:634:ASP:HB2	1.83	0.60
1:A:1063:LEU:HG	1:A:1065:LEU:H	1.63	0.60
1:A:1121:LEU:HB3	1:A:1124:GLU:HB2	1.83	0.60
1:A:459:PHE:HZ	1:A:482:ARG:HH12	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ASN:HA	1:A:990:TRP:HD1	1.66	0.60
1:A:1045:CYS:O	1:A:1049:GLU:N	2.34	0.60
1:A:1145:SER:O	1:A:1149:LYS:HG2	2.01	0.60
1:A:109:LEU:HA	1:A:612:ARG:HH21	1.65	0.60
1:A:135:ILE:HG21	1:A:492:CYS:CA	2.14	0.60
1:A:602:PHE:HE2	1:A:607:THR:H	1.49	0.60
1:A:905:ARG:NH2	1:A:991:LYS:O	2.32	0.60
1:A:947:ASP:CB	1:A:950:TYR:HB2	2.31	0.60
1:A:988:GLY:HA2	1:A:991:LYS:HE2	1.83	0.60
1:A:1252:ALA:CB	1:A:1273:ILE:HG21	2.32	0.60
1:A:1311:ARG:HB3	1:A:1339:GLN:HG2	1.83	0.60
1:A:988:GLY:O	1:A:991:LYS:HB3	2.02	0.60
1:A:1338:VAL:O	1:A:1341:THR:N	2.25	0.60
1:A:222:PRO:O	1:A:228:GLN:NE2	2.35	0.60
1:A:866:ARG:HG2	1:A:901:LEU:HD11	1.83	0.60
1:A:99:CYS:SG	1:A:131:ASP:HB2	2.42	0.60
1:A:475:GLY:H	3:A:1501:ATP:H5'2	1.66	0.60
1:A:217:HIS:O	1:A:221:PHE:N	2.35	0.59
1:A:412:THR:O	1:A:415:THR:OG1	2.20	0.59
1:A:632:ASN:C	1:A:635:LEU:HG	2.27	0.59
1:A:1147:LEU:O	1:A:1151:ILE:HG13	2.01	0.59
1:A:15:ILE:HG22	1:A:15:ILE:O	2.01	0.59
1:A:421:LEU:HD13	1:A:481:LYS:HB3	1.84	0.59
1:A:506:LEU:HD12	1:A:509:ILE:HD11	1.83	0.59
1:A:1279:VAL:HG23	1:A:1280:ILE:H	1.66	0.59
1:A:1397:PHE:O	1:A:1400:VAL:N	2.36	0.59
1:A:1235:ARG:HD2	1:A:1261:GLN:HB2	1.85	0.59
1:A:140:ILE:HG22	1:A:140:ILE:O	2.03	0.59
1:A:632:ASN:CA	1:A:635:LEU:HG	2.33	0.59
1:A:947:ASP:C	1:A:949:GLU:N	2.56	0.59
1:A:1015:ALA:HA	1:A:1018:GLN:HB2	1.83	0.59
1:A:1069:GLU:O	1:A:1073:LEU:N	2.21	0.59
1:A:1157:LEU:HD12	1:A:1159:VAL:H	1.67	0.59
1:A:907:HIS:HB2	1:A:908:PRO:CD	2.30	0.59
1:A:1033:ARG:HA	1:A:1059:SER:HB3	1.84	0.59
1:A:1135:SER:HB3	1:A:1163:LYS:HE3	1.85	0.59
1:A:1143:ASP:HB2	1:A:1146:LYS:HD3	1.85	0.59
1:A:196:GLN:HA	1:A:203:SER:HA	1.85	0.59
1:A:146:GLU:OE1	1:A:203:SER:N	2.36	0.58
1:A:214:TRP:CE3	1:A:231:LYS:HD2	2.38	0.58
1:A:1217:GLN:N	1:A:1244:THR:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:HA	2:C:495:ARG:HH11	1.66	0.58
1:A:468:VAL:HG21	1:A:578:LEU:HB3	1.85	0.58
1:A:917:LEU:N	1:A:1003:GLU:O	2.35	0.58
1:A:1321:PRO:HB3	1:A:1351:SER:CB	2.31	0.58
1:A:476:LYS:HZ1	1:A:582:HIS:HA	1.69	0.58
1:A:724:LEU:HD12	1:A:727:LEU:HD12	1.84	0.58
1:A:1388:ILE:HD13	2:C:465:ASN:ND2	2.19	0.58
1:A:477:THR:OG1	3:A:1501:ATP:O2B	2.20	0.58
1:A:645:VAL:O	1:A:649:CYS:N	2.35	0.58
1:A:1072:LEU:O	1:A:1075:THR:OG1	2.22	0.58
1:A:1248:ILE:CB	1:A:1273:ILE:HD11	2.31	0.58
1:A:1280:ILE:HG22	1:A:1284:ARG:CG	2.27	0.58
1:A:786:ILE:HD11	1:A:860:VAL:HG13	1.85	0.58
1:A:625:LEU:O	1:A:629:PHE:N	2.36	0.58
1:A:1273:ILE:O	1:A:1273:ILE:HG22	2.02	0.58
1:A:1301:MET:HG3	1:A:1304:LYS:HB2	1.86	0.58
1:A:99:CYS:SG	1:A:131:ASP:CB	2.92	0.57
1:A:137:LYS:HE3	1:A:140:ILE:CD1	2.30	0.57
1:A:196:GLN:NE2	1:A:201:GLY:O	2.31	0.57
1:A:1250:GLN:CD	1:A:1250:GLN:H	2.12	0.57
1:A:1292:GLN:O	1:A:1293:LYS:HG2	2.04	0.57
1:A:1359:LEU:HD22	1:A:1388:ILE:HG13	1.85	0.57
1:A:97:CYS:SG	1:A:102:LEU:HB3	2.45	0.57
1:A:570:ASN:O	1:A:573:SER:N	2.28	0.57
1:A:1069:GLU:HG3	1:A:1072:LEU:HD12	1.86	0.57
1:A:1357:ILE:HG21	2:C:462:GLU:HG3	1.86	0.57
1:A:506:LEU:HD12	1:A:509:ILE:CD1	2.35	0.57
1:A:673:GLN:O	1:A:676:SER:OG	2.19	0.57
1:A:1293:LYS:H	1:A:1322:ASN:ND2	2.01	0.57
1:A:949:GLU:O	1:A:952:SER:N	2.37	0.57
1:A:537:SER:O	1:A:541:GLN:N	2.37	0.57
1:A:956:HIS:N	1:A:959:GLU:OE1	2.37	0.57
1:A:217:HIS:HD2	1:A:227:LEU:HD22	1.70	0.57
1:A:832:MET:O	1:A:835:HIS:N	2.30	0.57
1:A:1082:LEU:HB3	1:A:1107:LEU:HD22	1.87	0.57
1:A:492:CYS:HB3	1:A:493:PRO:HD2	1.86	0.57
1:A:686:LEU:O	1:A:689:THR:OG1	2.19	0.57
1:A:1302:ASN:HA	1:A:1305:ILE:HD12	1.86	0.57
1:A:134:ASN:O	1:A:136:GLY:N	2.37	0.57
1:A:483:ILE:O	1:A:487:TRP:N	2.24	0.57
1:A:493:PRO:O	1:A:496:TYR:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LYS:HD3	1:A:417:ARG:NH2	2.19	0.57
1:A:788:SER:OG	1:A:789:PHE:N	2.37	0.57
1:A:1120:VAL:HG12	1:A:1121:LEU:HG	1.87	0.57
1:A:1252:ALA:HB3	1:A:1273:ILE:HG21	1.85	0.57
1:A:583:THR:HG21	1:A:731:LYS:HB2	1.85	0.57
1:A:635:LEU:HD12	1:A:636:GLN:CB	2.34	0.57
1:A:866:ARG:HE	1:A:901:LEU:HD21	1.69	0.57
1:A:59:SER:HA	1:A:132:VAL:HG11	1.87	0.56
1:A:502:PHE:O	1:A:549:LEU:N	2.38	0.56
1:A:602:PHE:HE2	1:A:607:THR:HG23	1.64	0.56
1:A:1050:LEU:HB2	1:A:1052:LYS:NZ	2.20	0.56
1:A:1065:LEU:O	1:A:1066:SER:HB3	2.04	0.56
1:A:1330:ARG:HH21	1:A:1332:ILE:HD11	1.70	0.56
2:C:457:SER:HA	2:C:460:ALA:HB3	1.87	0.56
1:A:44:LYS:HE2	1:A:105:PHE:HB2	1.86	0.56
1:A:169:TRP:CE3	1:A:170:PRO:HB3	2.40	0.56
1:A:465:VAL:O	1:A:466:MET:HG2	2.05	0.56
1:A:873:TYR:OH	1:A:904:PHE:N	2.38	0.56
1:A:956:HIS:CE1	1:A:1393:LEU:H	2.22	0.56
1:A:421:LEU:HD22	1:A:481:LYS:HD2	1.86	0.56
1:A:775:TYR:O	1:A:778:GLN:HG2	2.05	0.56
1:A:1212:ASN:HA	1:A:1241:LEU:HD12	1.87	0.56
1:A:1266:ARG:HA	1:A:1295:GLU:H	1.71	0.56
1:A:11:ARG:CD	1:A:53:PHE:CB	2.73	0.56
1:A:770:ASP:HA	1:A:773:LEU:HD12	1.87	0.56
1:A:43:HIS:O	1:A:47:MET:N	2.38	0.56
1:A:212:ASP:O	1:A:215:LYS:HB2	2.05	0.56
1:A:11:ARG:NH1	1:A:53:PHE:HD2	2.04	0.56
1:A:146:GLU:HA	1:A:149:LEU:HD12	1.86	0.56
1:A:1253:LYS:HD2	1:A:1257:ARG:NH2	2.21	0.56
1:A:1265:LEU:HD22	1:A:1291:PHE:HA	1.87	0.56
1:A:1217:GLN:O	1:A:1246:ASP:HB3	2.05	0.56
1:A:59:SER:OG	1:A:133:GLY:O	2.22	0.56
1:A:1331:ASN:HB3	1:A:1334:GLY:N	2.13	0.56
1:A:891:GLY:N	1:A:912:LEU:O	2.39	0.56
1:A:922:ASN:ND2	1:A:1008:ASN:HD22	2.03	0.56
1:A:1007:ASN:HD22	1:A:1035:PHE:HB2	1.70	0.56
1:A:1061:SER:O	1:A:1086:GLU:HB2	2.06	0.56
1:A:1388:ILE:CG2	2:C:465:ASN:OD1	2.54	0.56
1:A:141:ARG:HH21	1:A:205:GLY:HA3	1.71	0.55
1:A:406:GLN:NE2	1:A:499:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:CG	1:A:135:ILE:H	2.14	0.55
1:A:505:SER:HA	1:A:551:ASP:H	1.72	0.55
1:A:582:HIS:HE2	1:A:727:LEU:HB3	1.72	0.55
1:A:1095:PHE:HZ	1:A:1109:VAL:HG21	1.70	0.55
1:A:1132:GLU:HA	1:A:1157:LEU:HD13	1.89	0.55
1:A:11:ARG:CG	1:A:12:ILE:H	2.19	0.55
1:A:765:ARG:NH2	1:A:767:GLU:HB3	2.22	0.55
1:A:63:ARG:O	1:A:66:THR:OG1	2.15	0.55
1:A:955:GLU:O	1:A:1390:PHE:HB2	2.07	0.55
1:A:1091:PRO:HB2	1:A:1096:HIS:ND1	2.22	0.55
1:A:1252:ALA:CB	1:A:1273:ILE:CD1	2.84	0.55
1:A:1272:ASP:HA	1:A:1301:MET:SD	2.46	0.55
1:A:59:SER:CA	1:A:132:VAL:HG11	2.37	0.55
1:A:653:ILE:N	1:A:656:ALA:O	2.40	0.55
1:A:1280:ILE:HG22	1:A:1284:ARG:NE	2.21	0.55
1:A:11:ARG:CG	1:A:12:ILE:N	2.70	0.55
1:A:1154:PHE:HD1	1:A:1157:LEU:HD21	1.71	0.55
1:A:102:LEU:HD21	1:A:104:LEU:HD21	1.88	0.55
1:A:699:THR:HA	1:A:702:PHE:HB3	1.89	0.55
1:A:743:PHE:CE2	1:A:749:GLN:HB2	2.42	0.55
1:A:855:SER:HA	1:A:858:SER:HB3	1.89	0.55
1:A:1301:MET:HE2	1:A:1304:LYS:HG2	1.88	0.55
1:A:179:ARG:O	1:A:183:ALA:N	2.27	0.54
1:A:409:ASP:OD1	1:A:500:LEU:HD23	2.05	0.54
1:A:553:TYR:CE2	1:A:585:ARG:HG3	2.37	0.54
1:A:975:GLU:HA	1:A:978:ARG:NH2	2.18	0.54
1:A:1091:PRO:HA	1:A:1095:PHE:H	1.71	0.54
1:A:1245:GLY:HA2	1:A:1248:ILE:HD12	1.89	0.54
1:A:1293:LYS:HA	1:A:1322:ASN:HB3	1.89	0.54
1:A:132:VAL:CG1	1:A:133:GLY:H	2.20	0.54
1:A:162:ARG:HB2	1:A:187:VAL:HG22	1.89	0.54
1:A:1133:LYS:HE2	1:A:1161:HIS:CD2	2.39	0.54
1:A:32:PHE:CZ	1:A:974:TYR:HE1	2.25	0.54
1:A:635:LEU:CD1	1:A:636:GLN:HG2	2.29	0.54
1:A:553:TYR:N	1:A:553:TYR:CD1	2.73	0.54
1:A:76:TRP:CH2	1:A:116:ARG:NH1	2.70	0.54
1:A:459:PHE:HA	1:A:494:LEU:HD22	1.88	0.54
1:A:1202:LEU:HB3	1:A:1203:PRO:HD3	1.89	0.54
1:A:147:LYS:O	1:A:150:ARG:HG3	2.08	0.54
1:A:486:LEU:O	1:A:489:SER:N	2.40	0.54
1:A:137:LYS:HG2	1:A:493:PRO:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:ILE:HG12	1:A:1362:LEU:HB2	1.88	0.54
1:A:134:ASN:O	1:A:135:ILE:C	2.50	0.54
1:A:602:PHE:CD2	1:A:602:PHE:C	2.85	0.54
1:A:784:LYS:O	1:A:788:SER:OG	2.26	0.54
1:A:866:ARG:HE	1:A:901:LEU:CD2	2.20	0.54
1:A:1235:ARG:HB3	1:A:1262:LEU:HD23	1.90	0.54
1:A:1255:ILE:HG22	1:A:1255:ILE:O	2.07	0.54
1:A:476:LYS:HZ3	1:A:582:HIS:HA	1.73	0.53
1:A:579:ILE:HG22	1:A:581:VAL:CG2	2.38	0.53
1:A:1388:ILE:HD13	2:C:465:ASN:HD21	1.73	0.53
1:A:413:LYS:HB3	1:A:417:ARG:CZ	2.39	0.53
1:A:482:ARG:HH21	1:A:486:LEU:CD1	2.22	0.53
1:A:494:LEU:O	1:A:497:ARG:HG2	2.08	0.53
1:A:538:SER:HA	1:A:541:GLN:HB2	1.91	0.53
1:A:1211:LEU:H	1:A:1240:LEU:HA	1.73	0.53
1:A:1248:ILE:HG22	1:A:1252:ALA:HB2	1.90	0.53
1:A:1310:TYR:OH	1:A:1335:ARG:NH1	2.41	0.53
1:A:1325:GLU:OE2	1:A:1355:SER:OG	2.26	0.53
2:C:452:SER:C	2:C:454:ILE:H	2.17	0.53
1:A:11:ARG:HH11	1:A:53:PHE:HD2	1.57	0.53
1:A:141:ARG:HE	1:A:205:GLY:HA3	1.74	0.53
1:A:739:PRO:C	1:A:740:VAL:HG23	2.33	0.53
1:A:1065:LEU:HB3	1:A:1068:ALA:HB2	1.90	0.53
1:A:1276:ASP:C	1:A:1278:SER:H	2.16	0.53
1:A:77:THR:HG22	1:A:79:GLN:N	2.24	0.53
1:A:971:ILE:HG22	1:A:975:GLU:HG3	1.90	0.53
1:A:1246:ASP:H	1:A:1248:ILE:HG13	1.74	0.53
1:A:32:PHE:HB3	1:A:977:ILE:HG22	1.88	0.53
1:A:710:SER:HA	1:A:713:LEU:HD12	1.90	0.53
1:A:1007:ASN:C	1:A:1036:ASN:HB2	2.34	0.53
1:A:1017:LEU:O	1:A:1021:MET:N	2.41	0.53
1:A:1055:VAL:HG12	1:A:1056:THR:N	2.22	0.53
1:A:1071:GLU:O	1:A:1075:THR:N	2.34	0.53
1:A:1311:ARG:O	1:A:1315:GLN:N	2.41	0.53
2:C:477:THR:HA	2:C:480:LEU:HD12	1.91	0.53
1:A:135:ILE:HG23	1:A:493:PRO:N	2.22	0.53
1:A:161:ALA:HA	1:A:164:GLU:CD	2.34	0.53
1:A:826:SER:HB3	1:A:842:PHE:CE1	2.43	0.53
1:A:935:LYS:O	1:A:940:ASN:ND2	2.42	0.53
1:A:1301:MET:O	1:A:1305:ILE:HD12	2.09	0.53
1:A:1388:ILE:CG2	2:C:465:ASN:CG	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:H	1:A:235:GLU:CD	2.17	0.53
1:A:967:ASP:HB3	2:C:479:VAL:HG21	1.90	0.53
1:A:102:LEU:CD2	1:A:104:LEU:HG	2.39	0.53
1:A:130:LYS:HB3	1:A:172:TYR:OH	2.09	0.53
1:A:590:ARG:NH1	1:A:734:ALA:HB1	2.23	0.53
1:A:628:TYR:HA	1:A:635:LEU:CD2	2.38	0.53
1:A:873:TYR:CE1	1:A:877:THR:HG21	2.44	0.53
1:A:1048:LEU:HA	1:A:1052:LYS:NZ	2.24	0.53
1:A:1359:LEU:CD1	1:A:1388:ILE:HD11	2.28	0.53
1:A:1375:ASN:HD21	1:A:1383:GLN:HG3	1.71	0.53
1:A:465:VAL:CG1	1:A:466:MET:N	2.72	0.52
1:A:11:ARG:CD	1:A:53:PHE:HB3	2.24	0.52
1:A:188:PHE:CZ	1:A:190:GLY:HA2	2.44	0.52
1:A:450:GLN:N	1:A:450:GLN:OE1	2.43	0.52
1:A:135:ILE:HG23	1:A:493:PRO:CD	2.40	0.52
1:A:235:GLU:HA	1:A:238:GLN:OE1	2.10	0.52
1:A:237:ALA:O	1:A:240:ILE:HG22	2.08	0.52
1:A:1111:LEU:HD23	1:A:1114:LYS:HD2	1.92	0.52
1:A:214:TRP:HZ3	1:A:231:LYS:HB2	1.73	0.52
1:A:780:ASP:O	1:A:815:LEU:HD11	2.10	0.52
1:A:898:VAL:HA	1:A:901:LEU:HB3	1.91	0.52
1:A:1229:GLN:O	1:A:1233:SER:N	2.37	0.52
1:A:602:PHE:CE2	1:A:607:THR:CG2	2.89	0.52
1:A:972:LYS:HE3	1:A:976:ASN:HD21	1.75	0.52
1:A:1356:LEU:O	1:A:1384:SER:HA	2.09	0.52
1:A:1388:ILE:CG2	1:A:1389:ILE:H	2.19	0.52
1:A:498:PHE:CD1	1:A:545:GLN:HA	2.39	0.52
1:A:1217:GLN:HG2	1:A:1248:ILE:HD11	1.91	0.52
1:A:558:SER:HA	1:A:563:LEU:HD22	1.91	0.52
1:A:1260:LEU:HD21	1:A:1285:ALA:HB1	1.92	0.52
1:A:1283:ALA:HA	1:A:1286:ALA:HB3	1.91	0.52
1:A:1327:ASN:OD1	1:A:1357:ILE:HB	2.10	0.52
1:A:632:ASN:HA	1:A:635:LEU:CD2	2.40	0.52
1:A:1092:GLU:HG3	1:A:1096:HIS:CE1	2.45	0.52
2:C:452:SER:O	2:C:453:ARG:HG2	2.10	0.52
1:A:553:TYR:N	1:A:553:TYR:HD1	2.07	0.52
1:A:935:LYS:HA	1:A:938:PHE:CE2	2.45	0.52
1:A:1125:PHE:CZ	1:A:1149:LYS:HA	2.45	0.51
1:A:1293:LYS:H	1:A:1322:ASN:HD22	1.56	0.51
1:A:1307:GLU:H	1:A:1307:GLU:CD	2.18	0.51
1:A:443:LYS:N	1:A:596:SER:HB2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:PHE:CE2	1:A:606:ASN:HB2	2.44	0.51
1:A:602:PHE:CZ	1:A:606:ASN:CB	2.93	0.51
1:A:643:LEU:HA	1:A:646:ALA:HB3	1.91	0.51
1:A:739:PRO:O	1:A:740:VAL:CG2	2.57	0.51
1:A:1097:ASN:H	1:A:1123:ARG:HH11	1.58	0.51
1:A:1301:MET:HE2	1:A:1304:LYS:H	1.75	0.51
1:A:761:LEU:HD11	1:A:776:LEU:HD11	1.91	0.51
1:A:765:ARG:HE	1:A:768:ASP:CG	2.19	0.51
1:A:832:MET:HB3	1:A:838:THR:HG21	1.92	0.51
1:A:1015:ALA:O	1:A:1019:VAL:N	2.32	0.51
1:A:1042:GLU:HG3	1:A:1068:ALA:HA	1.92	0.51
1:A:32:PHE:CE1	1:A:978:ARG:HG2	2.45	0.51
1:A:84:ALA:HB1	1:A:86:PHE:CE1	2.45	0.51
1:A:170:PRO:HB2	1:A:174:HIS:H	1.75	0.51
1:A:553:TYR:CE2	1:A:585:ARG:CZ	2.91	0.51
1:A:96:GLN:HA	1:A:103:ILE:HG12	1.93	0.51
1:A:123:GLU:HG3	1:A:124:CYS:N	2.24	0.51
1:A:476:LYS:HB2	3:A:1501:ATP:O3A	2.10	0.51
1:A:939:GLU:O	1:A:942:GLN:HG2	2.10	0.51
1:A:982:LEU:HD21	1:A:1016:LEU:HB3	1.92	0.51
1:A:1071:GLU:O	1:A:1075:THR:HG23	2.11	0.51
1:A:1388:ILE:HG22	1:A:1389:ILE:H	1.71	0.51
1:A:743:PHE:HE2	1:A:749:GLN:HB2	1.76	0.51
1:A:885:ILE:O	1:A:889:LEU:HG	2.09	0.51
1:A:1272:ASP:CG	1:A:1273:ILE:H	2.19	0.51
1:A:1136:ILE:HG22	1:A:1137:GLN:N	2.26	0.51
1:A:1147:LEU:O	1:A:1150:PHE:N	2.44	0.51
1:A:108:SER:HA	2:C:495:ARG:NH1	2.26	0.51
1:A:1144:LEU:HD23	1:A:1147:LEU:HD12	1.93	0.51
1:A:1232:GLY:HA2	1:A:1235:ARG:NE	2.26	0.51
1:A:902:GLN:HB3	1:A:905:ARG:H	1.76	0.51
1:A:523:LEU:HB3	1:A:525:GLY:O	2.11	0.50
1:A:810:SER:HB2	1:A:884:PHE:CE2	2.46	0.50
1:A:1274:LEU:HD11	1:A:1299:ILE:CG2	2.29	0.50
1:A:1055:VAL:HG13	1:A:1078:ALA:O	2.11	0.50
1:A:1110:ARG:C	1:A:1111:LEU:HD12	2.36	0.50
1:A:1217:GLN:HB2	1:A:1243:PRO:HB2	1.93	0.50
1:A:1391:TRP:CZ3	1:A:1393:LEU:HB3	2.46	0.50
1:A:32:PHE:CD1	1:A:978:ARG:HG2	2.46	0.50
2:C:467:SER:O	2:C:471:ILE:HG13	2.11	0.50
1:A:445:ILE:HD11	1:A:594:GLY:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ILE:HG21	1:A:518:ILE:HD13	1.93	0.50
1:A:632:ASN:HA	1:A:635:LEU:HD21	1.92	0.50
1:A:877:THR:O	1:A:881:CYS:HB2	2.12	0.50
1:A:443:LYS:HB2	1:A:598:GLU:OE2	2.12	0.50
1:A:512:ASP:O	1:A:559:LEU:CD2	2.60	0.50
1:A:559:LEU:H	1:A:563:LEU:HB3	1.76	0.50
1:A:778:GLN:O	1:A:784:LYS:NZ	2.34	0.50
1:A:1242:VAL:HG21	1:A:1270:PHE:CE1	2.46	0.50
1:A:219:LYS:HD2	1:A:220:TRP:NE1	2.27	0.50
1:A:735:GLN:HB2	1:A:737:LEU:O	2.12	0.50
1:A:950:TYR:CZ	1:A:954:PHE:HZ	2.30	0.50
1:A:984:ASP:OD1	1:A:988:GLY:N	2.45	0.50
1:A:1070:GLN:O	1:A:1073:LEU:HB3	2.12	0.50
1:A:1195:ALA:HA	1:A:1198:PHE:HB2	1.93	0.50
1:A:582:HIS:NE2	1:A:727:LEU:HB3	2.26	0.50
1:A:873:TYR:CZ	1:A:903:TYR:CD2	2.99	0.50
2:C:491:LEU:O	2:C:495:ARG:N	2.44	0.50
1:A:234:GLU:HG3	1:A:238:GLN:NE2	2.27	0.50
1:A:602:PHE:CE1	1:A:642:PRO:HB3	2.46	0.50
1:A:786:ILE:CD1	1:A:860:VAL:HG13	2.42	0.50
1:A:1033:ARG:C	1:A:1034:LEU:HD12	2.36	0.50
1:A:1068:ALA:O	1:A:1071:GLU:N	2.42	0.50
1:A:1379:GLU:HB3	1:A:1381:HIS:CE1	2.46	0.50
1:A:1388:ILE:CD1	2:C:465:ASN:ND2	2.75	0.50
1:A:1066:SER:H	1:A:1093:GLN:HE21	1.59	0.50
1:A:1210:ILE:HG12	1:A:1239:GLU:CG	2.41	0.50
1:A:188:PHE:CE2	1:A:190:GLY:HA2	2.46	0.49
1:A:246:PHE:CD2	1:A:247:VAL:HG13	2.47	0.49
1:A:798:SER:OG	1:A:799:HIS:N	2.45	0.49
1:A:1224:SER:O	1:A:1228:ALA:N	2.25	0.49
1:A:187:VAL:O	1:A:195:VAL:HA	2.12	0.49
1:A:1110:ARG:NH1	1:A:1135:SER:HB2	2.27	0.49
1:A:1227:PHE:CE2	1:A:1231:LEU:HD22	2.47	0.49
1:A:212:ASP:HB2	1:A:215:LYS:HG3	1.95	0.49
1:A:462:LEU:C	1:A:463:ASN:HD22	2.20	0.49
1:A:519:ILE:O	1:A:522:GLN:N	2.45	0.49
1:A:1045:CYS:O	1:A:1049:GLU:HG3	2.12	0.49
1:A:1138:THR:OG1	1:A:1166:PHE:O	2.22	0.49
1:A:1225:GLU:O	1:A:1229:GLN:N	2.39	0.49
1:A:1241:LEU:HD23	1:A:1269:THR:HG21	1.94	0.49
1:A:651:ASP:O	1:A:656:ALA:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ARG:HH22	2:C:435:LYS:HE3	1.76	0.49
1:A:1132:GLU:OE2	1:A:1158:HIS:ND1	2.45	0.49
1:A:1138:THR:HG21	1:A:1167:LEU:HD12	1.94	0.49
1:A:134:ASN:C	1:A:136:GLY:N	2.69	0.49
1:A:142:VAL:C	1:A:145:PRO:HD2	2.37	0.49
1:A:196:GLN:HE21	1:A:201:GLY:C	2.21	0.49
1:A:771:LEU:O	1:A:774:TYR:HB3	2.12	0.49
1:A:1024:PHE:O	1:A:1027:SER:OG	2.24	0.49
1:A:1193:PHE:CE2	1:A:1217:GLN:HA	2.43	0.49
1:A:1199:VAL:HB	1:A:1226:LYS:HB3	1.93	0.49
1:A:1207:SER:HA	1:A:1236:ASN:HD22	1.77	0.49
1:A:1239:GLU:HB2	1:A:1267:VAL:HB	1.94	0.49
1:A:1308:GLU:HA	1:A:1311:ARG:HH12	1.77	0.49
1:A:169:TRP:CZ3	1:A:170:PRO:HB3	2.48	0.49
1:A:115:GLU:HB3	1:A:119:LYS:HE3	1.93	0.49
1:A:628:TYR:CD1	1:A:635:LEU:HB2	2.47	0.49
1:A:1040:PHE:CD2	1:A:1044:ILE:HD11	2.47	0.49
1:A:1314:PHE:CD2	1:A:1346:LEU:HD21	2.48	0.49
1:A:11:ARG:CD	1:A:53:PHE:HB2	2.35	0.49
1:A:166:PHE:CD2	1:A:178:PRO:HB3	2.48	0.49
1:A:225:GLU:O	1:A:229:SER:N	2.35	0.49
1:A:888:PHE:O	1:A:892:LYS:NZ	2.35	0.49
1:A:1294:LEU:O	1:A:1323:LEU:HD23	2.13	0.49
1:A:468:VAL:HB	1:A:579:ILE:O	2.13	0.49
1:A:1210:ILE:HG22	1:A:1211:LEU:N	2.28	0.49
1:A:244:GLU:HG2	1:A:245:GLY:N	2.28	0.48
1:A:628:TYR:C	1:A:635:LEU:CD2	2.64	0.48
1:A:951:THR:O	1:A:954:PHE:N	2.42	0.48
1:A:1090:LEU:O	1:A:1093:GLN:HB2	2.13	0.48
1:A:1391:TRP:CE3	1:A:1393:LEU:HB3	2.48	0.48
1:A:99:CYS:HB3	1:A:124:CYS:SG	2.53	0.48
1:A:218:ALA:HA	1:A:221:PHE:O	2.13	0.48
1:A:1097:ASN:HB3	1:A:1100:LYS:HD2	1.95	0.48
1:A:1307:GLU:HG2	1:A:1337:GLN:HG3	1.95	0.48
1:A:47:MET:HB3	1:A:51:LYS:NZ	2.28	0.48
1:A:159:GLU:HA	1:A:162:ARG:HG2	1.95	0.48
1:A:607:THR:OG1	1:A:608:VAL:N	2.46	0.48
1:A:1118:LEU:HD22	1:A:1145:SER:OG	2.13	0.48
1:A:1133:LYS:HA	1:A:1160:PHE:O	2.13	0.48
1:A:168:ASP:HB2	1:A:188:PHE:HE2	1.78	0.48
1:A:509:ILE:CG2	1:A:518:ILE:HG12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:GLY:C	1:A:991:LYS:HB3	2.38	0.48
1:A:1069:GLU:CG	1:A:1072:LEU:HD12	2.44	0.48
1:A:153:LYS:NZ	1:A:156:TYR:HB2	2.28	0.48
1:A:459:PHE:HB3	1:A:494:LEU:CB	2.39	0.48
1:A:894:LEU:O	1:A:916:SER:N	2.35	0.48
1:A:1076:LEU:HD22	1:A:1101:PHE:CD1	2.48	0.48
1:A:1095:PHE:CD2	1:A:1120:VAL:HG13	2.48	0.48
1:A:1162:LEU:HD21	1:A:1164:CYS:SG	2.53	0.48
1:A:1201:ILE:HA	1:A:1204:ASN:OD1	2.14	0.48
1:A:1365:LEU:HA	1:A:1368:GLU:HB2	1.96	0.48
1:A:851:VAL:HG11	2:C:441:GLN:HB3	1.94	0.48
1:A:1280:ILE:HG22	1:A:1284:ARG:HE	1.79	0.48
1:A:1375:ASN:ND2	1:A:1383:GLN:CG	2.65	0.48
1:A:86:PHE:HA	1:A:96:GLN:O	2.14	0.48
1:A:706:PHE:HA	1:A:708:PHE:CZ	2.49	0.48
1:A:731:LYS:HE3	1:A:742:ARG:HG2	1.95	0.48
1:A:925:LYS:O	1:A:926:MET:HG2	2.14	0.48
1:A:1045:CYS:HB2	1:A:1046:PRO:HD3	1.96	0.48
1:A:1225:GLU:HG2	1:A:1229:GLN:HG2	1.96	0.48
1:A:245:GLY:HA2	1:A:463:ASN:HD21	1.76	0.48
1:A:471:GLU:O	1:A:476:LYS:NZ	2.46	0.47
1:A:632:ASN:HA	1:A:635:LEU:HG	1.96	0.47
1:A:1031:GLU:HG3	1:A:1056:THR:HB	1.95	0.47
2:C:452:SER:O	2:C:454:ILE:N	2.46	0.47
2:C:457:SER:O	2:C:461:THR:OG1	2.30	0.47
1:A:76:TRP:CD1	1:A:107:ASN:HB3	2.49	0.47
1:A:887:GLN:HA	1:A:890:ARG:CZ	2.44	0.47
1:A:1161:HIS:ND1	1:A:1184:ARG:HB2	2.29	0.47
1:A:1135:SER:CB	1:A:1163:LYS:HE3	2.44	0.47
1:A:1359:LEU:HD13	1:A:1388:ILE:CG1	2.44	0.47
1:A:886:LEU:HA	1:A:889:LEU:HD12	1.96	0.47
1:A:950:TYR:HE1	1:A:1362:LEU:HD13	1.80	0.47
1:A:1320:LEU:C	1:A:1322:ASN:H	2.22	0.47
1:A:482:ARG:HH21	1:A:486:LEU:HD11	1.78	0.47
1:A:873:TYR:CZ	1:A:903:TYR:HD2	2.33	0.47
1:A:30:ASP:HB3	1:A:626:ILE:HD13	1.96	0.47
1:A:78:PRO:HD2	1:A:605:TYR:CE1	2.50	0.47
1:A:97:CYS:HB3	1:A:100:CYS:HB2	1.96	0.47
1:A:140:ILE:O	1:A:140:ILE:CG2	2.63	0.47
1:A:464:SER:O	1:A:576:CYS:CA	2.56	0.47
1:A:627:ILE:O	1:A:630:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:PRO:C	1:A:1234:LEU:HD13	2.39	0.47
1:A:738:ARG:HB3	1:A:739:PRO:HD3	1.96	0.47
1:A:861:SER:HB3	1:A:894:LEU:HD21	1.97	0.47
1:A:949:GLU:OE1	1:A:1364:TRP:HA	2.15	0.47
1:A:556:LEU:HD12	1:A:556:LEU:C	2.38	0.47
1:A:1058:CYS:SG	1:A:1060:MET:HE3	2.55	0.47
1:A:695:GLN:HA	1:A:698:LEU:HG	1.97	0.47
1:A:1254:LEU:CD2	1:A:1257:ARG:HD2	2.44	0.47
1:A:1283:ALA:O	1:A:1287:THR:N	2.26	0.47
1:A:1297:LEU:O	1:A:1326:LEU:HA	2.15	0.47
1:A:19:PHE:HZ	2:C:495:ARG:HH12	1.62	0.46
1:A:33:GLN:HB3	1:A:977:ILE:HG23	1.96	0.46
1:A:411:TYR:O	1:A:415:THR:HG23	2.15	0.46
1:A:576:CYS:C	1:A:577:LEU:HD12	2.40	0.46
1:A:873:TYR:CE2	1:A:903:TYR:CB	2.94	0.46
1:A:36:LYS:HG3	1:A:977:ILE:HG12	1.96	0.46
1:A:442:SER:O	1:A:451:GLU:HB3	2.15	0.46
1:A:466:MET:HB2	1:A:578:LEU:HD23	1.98	0.46
1:A:905:ARG:NE	1:A:991:LYS:HA	2.30	0.46
1:A:927:SER:O	1:A:930:VAL:HG22	2.15	0.46
1:A:1038:SER:O	1:A:1065:LEU:HB2	2.13	0.46
1:A:1225:GLU:HA	1:A:1228:ALA:HB3	1.96	0.46
1:A:1350:VAL:C	1:A:1351:SER:HG	2.10	0.46
1:A:404:SER:OG	1:A:407:LEU:HB2	2.14	0.46
1:A:417:ARG:NE	1:A:488:ALA:HB1	2.24	0.46
1:A:467:CYS:SG	1:A:596:SER:HA	2.56	0.46
1:A:635:LEU:CG	1:A:636:GLN:N	2.77	0.46
1:A:1016:LEU:O	1:A:1019:VAL:HB	2.16	0.46
1:A:1076:LEU:N	1:A:1077:PRO:HD3	2.30	0.46
1:A:1280:ILE:CG2	1:A:1284:ARG:HE	2.29	0.46
2:C:435:LYS:HD2	2:C:482:GLN:HE22	1.81	0.46
1:A:510:THR:OG1	1:A:511:PRO:HD3	2.15	0.46
1:A:1033:ARG:HG2	1:A:1059:SER:HB3	1.98	0.46
2:C:450:SER:HB3	2:C:453:ARG:N	2.31	0.46
1:A:85:GLY:HA3	1:A:98:PHE:HE1	1.81	0.46
1:A:648:VAL:O	1:A:651:ASP:N	2.48	0.46
1:A:1117:VAL:HA	1:A:1120:VAL:HG23	1.96	0.46
1:A:1241:LEU:HA	1:A:1269:THR:OG1	2.15	0.46
1:A:465:VAL:O	1:A:466:MET:CG	2.64	0.46
1:A:1089:GLN:NE2	1:A:1094:LEU:HB3	2.26	0.46
1:A:1210:ILE:CG2	1:A:1211:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:GLU:O	1:A:1226:LYS:N	2.30	0.46
1:A:74:ARG:HA	1:A:74:ARG:HD3	1.73	0.46
1:A:822:LEU:CD1	1:A:825:MET:HG2	2.45	0.46
1:A:882:SER:O	1:A:886:LEU:HG	2.15	0.46
2:C:435:LYS:HD2	2:C:482:GLN:NE2	2.31	0.46
2:C:450:SER:O	2:C:453:ARG:HB3	2.15	0.46
1:A:115:GLU:O	1:A:119:LYS:N	2.31	0.46
1:A:962:ARG:NH2	1:A:966:GLN:OE1	2.48	0.46
1:A:100:CYS:SG	1:A:117:HIS:NE2	2.59	0.46
1:A:182:SER:C	1:A:185:GLY:H	2.23	0.46
1:A:788:SER:HG	1:A:789:PHE:H	1.62	0.46
1:A:1331:ASN:ND2	1:A:1335:ARG:HB2	2.30	0.46
2:C:477:THR:HA	2:C:480:LEU:HB2	1.98	0.46
1:A:459:PHE:CA	1:A:494:LEU:HD22	2.46	0.45
1:A:1017:LEU:O	1:A:1020:LEU:N	2.49	0.45
1:A:1223:THR:HA	1:A:1226:LYS:HD2	1.97	0.45
1:A:1393:LEU:HD12	1:A:1395:VAL:H	1.82	0.45
1:A:126:PHE:O	1:A:128:GLN:HG3	2.16	0.45
1:A:459:PHE:HZ	1:A:482:ARG:NH1	2.13	0.45
1:A:630:ILE:HG21	2:C:427:SER:HB3	1.97	0.45
1:A:1048:LEU:HD23	1:A:1052:LYS:HE2	1.98	0.45
1:A:102:LEU:HD21	1:A:104:LEU:CD2	2.46	0.45
1:A:160:GLU:O	1:A:164:GLU:HG3	2.16	0.45
1:A:676:SER:OG	1:A:677:LEU:N	2.50	0.45
1:A:777:ARG:HA	1:A:811:HIS:NE2	2.31	0.45
1:A:788:SER:CB	1:A:832:MET:HE1	2.46	0.45
1:A:1310:TYR:HB2	1:A:1339:GLN:OE1	2.16	0.45
1:A:559:LEU:O	1:A:560:PRO:C	2.59	0.45
1:A:913:LEU:C	1:A:914:LEU:HD12	2.42	0.45
1:A:918:LYS:HD3	2:C:440:GLY:HA2	1.99	0.45
1:A:1147:LEU:C	1:A:1151:ILE:HG13	2.41	0.45
1:A:582:HIS:CD2	1:A:727:LEU:HD13	2.51	0.45
1:A:887:GLN:HA	1:A:890:ARG:NE	2.32	0.45
1:A:1102:LEU:HD23	1:A:1102:LEU:HA	1.71	0.45
1:A:1110:ARG:HH12	1:A:1163:LYS:HB3	1.81	0.45
1:A:1136:ILE:O	1:A:1164:CYS:HA	2.17	0.45
1:A:1332:ILE:HB	1:A:1333:PRO:HD3	1.99	0.45
1:A:478:THR:HA	1:A:481:LYS:HE2	1.99	0.45
1:A:593:LEU:HD23	1:A:593:LEU:C	2.41	0.45
1:A:707:GLU:HG2	1:A:708:PHE:N	2.32	0.45
1:A:954:PHE:HA	1:A:1390:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:VAL:HA	1:A:1296:ASN:HB2	1.99	0.45
1:A:63:ARG:HD2	1:A:87:TYR:HA	1.97	0.45
1:A:487:TRP:HA	1:A:495:LEU:HD13	1.97	0.45
1:A:502:PHE:HD2	1:A:548:PHE:CE1	2.34	0.45
1:A:671:TYR:O	1:A:674:TYR:HB3	2.16	0.45
1:A:786:ILE:C	1:A:790:ASN:HB2	2.41	0.45
1:A:905:ARG:HG2	1:A:990:TRP:O	2.16	0.45
1:A:1075:THR:OG1	1:A:1077:PRO:HD3	2.17	0.45
1:A:1079:LEU:O	1:A:1104:LEU:HD12	2.17	0.45
1:A:1132:GLU:HG2	1:A:1158:HIS:H	1.81	0.45
1:A:1313:PHE:HD2	1:A:1314:PHE:CD1	2.35	0.45
1:A:515:LEU:HB3	1:A:517:ASN:H	1.82	0.45
1:A:1095:PHE:HA	1:A:1098:LEU:HB2	1.99	0.45
1:A:1310:TYR:CZ	1:A:1335:ARG:NH1	2.85	0.45
1:A:108:SER:HB2	1:A:111:LYS:HB2	1.99	0.45
1:A:213:PRO:O	1:A:216:GLU:N	2.49	0.45
1:A:484:ALA:O	1:A:487:TRP:N	2.50	0.45
1:A:1121:LEU:HD13	1:A:1124:GLU:HB2	1.98	0.45
1:A:1161:HIS:HB3	1:A:1185:GLU:CD	2.42	0.45
2:C:450:SER:HB3	2:C:453:ARG:CA	2.47	0.45
1:A:59:SER:HA	1:A:132:VAL:CG2	2.47	0.45
1:A:775:TYR:O	1:A:778:GLN:N	2.31	0.45
1:A:892:LYS:O	1:A:914:LEU:N	2.49	0.45
1:A:899:LEU:HD13	1:A:991:LYS:HD3	1.99	0.45
1:A:1219:PRO:HA	1:A:1246:ASP:OD2	2.16	0.45
1:A:1227:PHE:CZ	1:A:1231:LEU:HD22	2.52	0.45
1:A:515:LEU:HD13	1:A:517:ASN:OD1	2.17	0.44
1:A:685:PRO:O	1:A:689:THR:HG23	2.17	0.44
1:A:1343:VAL:HA	1:A:1346:LEU:CG	2.38	0.44
1:A:19:PHE:HE1	1:A:108:SER:OG	1.97	0.44
1:A:59:SER:HA	1:A:132:VAL:HG13	1.87	0.44
1:A:454:THR:O	1:A:458:VAL:HG23	2.17	0.44
1:A:459:PHE:HZ	1:A:482:ARG:NH2	2.14	0.44
1:A:512:ASP:O	1:A:559:LEU:HD21	2.17	0.44
1:A:548:PHE:C	1:A:549:LEU:HD12	2.42	0.44
1:A:643:LEU:O	1:A:647:ALA:N	2.42	0.44
1:A:694:GLY:C	1:A:756:ARG:HG2	2.42	0.44
1:A:761:LEU:O	1:A:804:ALA:HB2	2.17	0.44
1:A:1055:VAL:HG12	1:A:1080:GLN:HG3	1.98	0.44
1:A:1245:GLY:HA3	1:A:1272:ASP:OD2	2.17	0.44
1:A:138:TYR:HD2	1:A:220:TRP:CZ2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD22	1:A:189:THR:HG21	1.99	0.44
1:A:245:GLY:CA	1:A:463:ASN:ND2	2.72	0.44
1:A:1266:ARG:HA	1:A:1294:LEU:HD12	1.98	0.44
1:A:1305:ILE:HG23	1:A:1335:ARG:HH11	1.82	0.44
1:A:1367:ASP:O	1:A:1370:ASP:HB2	2.17	0.44
1:A:135:ILE:C	1:A:493:PRO:HD3	2.42	0.44
1:A:593:LEU:HD23	1:A:594:GLY:N	2.33	0.44
1:A:960:TRP:CD1	2:C:472:LEU:HD12	2.52	0.44
1:A:1230:ALA:HA	1:A:1233:SER:HB3	1.98	0.44
1:A:1253:LYS:O	1:A:1257:ARG:HG3	2.17	0.44
1:A:463:ASN:O	1:A:466:MET:HE2	2.17	0.44
1:A:1018:GLN:O	1:A:1021:MET:HB3	2.16	0.44
1:A:1184:ARG:HA	1:A:1208:LEU:HD12	2.00	0.44
1:A:233:SER:N	1:A:235:GLU:OE1	2.50	0.44
1:A:486:LEU:HB3	1:A:495:LEU:HD11	1.98	0.44
1:A:600:GLN:HG2	1:A:601:GLU:HG2	1.99	0.44
1:A:766:GLN:O	1:A:769:GLN:HG2	2.17	0.44
1:A:781:SER:O	1:A:815:LEU:HD21	2.17	0.44
1:A:1148:VAL:HA	1:A:1151:ILE:HD12	2.00	0.44
2:C:459:TYR:O	2:C:463:VAL:HG23	2.18	0.44
1:A:465:VAL:HG12	1:A:466:MET:N	2.32	0.44
1:A:695:GLN:O	1:A:698:LEU:HB2	2.18	0.44
1:A:988:GLY:CA	1:A:991:LYS:HE2	2.47	0.44
1:A:933:SER:HA	1:A:936:THR:HG23	2.00	0.44
1:A:956:HIS:HB3	1:A:1392:LYS:HB3	1.98	0.44
1:A:982:LEU:CD2	1:A:1016:LEU:HB3	2.48	0.44
1:A:991:LYS:O	1:A:994:PRO:HD2	2.18	0.44
1:A:1091:PRO:HB3	1:A:1095:PHE:HB2	2.00	0.44
1:A:79:GLN:HA	1:A:82:ALA:HB2	2.00	0.44
2:C:455:GLU:O	2:C:458:ASP:HB2	2.18	0.44
1:A:244:GLU:HG2	1:A:245:GLY:H	1.83	0.43
1:A:667:LEU:O	1:A:670:SER:OG	2.29	0.43
1:A:946:ILE:HG22	1:A:947:ASP:N	2.24	0.43
1:A:1001:LYS:HA	1:A:1029:SER:OG	2.17	0.43
1:A:1136:ILE:CG2	1:A:1137:GLN:N	2.80	0.43
1:A:1265:LEU:HD21	1:A:1291:PHE:CD1	2.52	0.43
1:A:1298:ASP:C	1:A:1299:ILE:HG13	2.43	0.43
2:C:477:THR:HG22	2:C:480:LEU:HD12	1.99	0.43
1:A:174:HIS:O	1:A:174:HIS:CG	2.72	0.43
1:A:1035:PHE:HA	1:A:1061:SER:OG	2.18	0.43
1:A:1143:ASP:O	1:A:1146:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:ILE:CG2	1:A:1273:ILE:HD11	2.48	0.43
1:A:1298:ASP:OD1	1:A:1327:ASN:HB2	2.17	0.43
1:A:141:ARG:HB2	1:A:142:VAL:HG23	2.00	0.43
1:A:627:ILE:HD13	1:A:663:GLN:H	1.83	0.43
1:A:720:GLU:HA	1:A:722:GLU:HG2	2.01	0.43
1:A:921:ILE:HB	1:A:1010:ASP:HB2	2.00	0.43
1:A:1078:ALA:HB1	1:A:1104:LEU:HD11	2.00	0.43
1:A:1094:LEU:HD23	1:A:1095:PHE:CE1	2.53	0.43
1:A:1146:LYS:O	1:A:1149:LYS:HB2	2.17	0.43
1:A:1167:LEU:HD11	1:A:1173:LEU:HD21	2.01	0.43
1:A:1279:VAL:HG23	1:A:1280:ILE:N	2.32	0.43
1:A:462:LEU:HD11	1:A:576:CYS:HB2	1.99	0.43
1:A:557:ALA:O	1:A:563:LEU:HD22	2.18	0.43
1:A:1302:ASN:O	1:A:1305:ILE:HB	2.18	0.43
2:C:462:GLU:HA	2:C:465:ASN:HB2	2.01	0.43
1:A:100:CYS:HG	1:A:117:HIS:CD2	2.28	0.43
1:A:235:GLU:O	1:A:239:TYR:HD1	2.01	0.43
1:A:520:CYS:HA	1:A:523:LEU:CB	2.44	0.43
1:A:850:LEU:HD21	2:C:470:GLN:HG2	2.00	0.43
1:A:877:THR:HA	1:A:881:CYS:SG	2.58	0.43
1:A:1161:HIS:N	1:A:1183:LEU:HD22	2.33	0.43
1:A:1200:ASN:O	1:A:1203:PRO:HD2	2.18	0.43
1:A:1274:LEU:O	1:A:1276:ASP:N	2.52	0.43
1:A:135:ILE:CA	1:A:493:PRO:HD3	2.49	0.43
1:A:135:ILE:HA	1:A:493:PRO:HD3	1.99	0.43
1:A:144:ARG:NE	1:A:496:TYR:OH	2.51	0.43
1:A:1064:GLU:HB3	1:A:1069:GLU:OE2	2.18	0.43
1:A:1244:THR:HG22	1:A:1271:HIS:HB2	2.00	0.43
1:A:1309:GLY:HA2	1:A:1312:ASN:ND2	2.33	0.43
1:A:106:GLY:O	1:A:116:ARG:NH1	2.52	0.43
1:A:477:THR:H	3:A:1501:ATP:PA	2.41	0.43
1:A:743:PHE:HZ	1:A:752:LEU:HD12	1.83	0.43
1:A:1031:GLU:N	1:A:1031:GLU:OE1	2.51	0.43
1:A:514:GLY:CA	1:A:518:ILE:HD11	2.49	0.43
1:A:606:ASN:HA	1:A:609:SER:HB3	2.01	0.43
1:A:852:SER:OG	1:A:855:SER:HB3	2.18	0.43
1:A:944:PRO:HB3	1:A:950:TYR:HE2	1.83	0.43
1:A:1150:PHE:HB3	1:A:1154:PHE:CE2	2.54	0.43
1:A:1378:LYS:HG3	1:A:1379:GLU:HG3	2.01	0.43
1:A:508:SER:O	1:A:511:PRO:HD2	2.19	0.43
1:A:629:PHE:HD1	1:A:629:PHE:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LEU:HD23	1:A:748:PHE:CD2	2.53	0.43
1:A:840:LEU:HD22	2:C:480:LEU:HB3	2.01	0.43
1:A:1090:LEU:HB2	1:A:1093:GLN:CG	2.46	0.43
1:A:1099:HIS:O	1:A:1102:LEU:N	2.52	0.43
1:A:1123:ARG:O	1:A:1126:PRO:HD2	2.19	0.43
1:A:1253:LYS:HG3	1:A:1254:LEU:N	2.34	0.43
1:A:97:CYS:HB2	1:A:102:LEU:N	2.34	0.42
1:A:140:ILE:O	1:A:145:PRO:HG2	2.18	0.42
1:A:212:ASP:HB2	1:A:215:LYS:CG	2.49	0.42
1:A:456:PRO:HA	1:A:459:PHE:CD2	2.54	0.42
1:A:602:PHE:CE2	1:A:607:THR:N	2.87	0.42
1:A:765:ARG:HD2	1:A:765:ARG:HA	1.78	0.42
1:A:951:THR:HG23	1:A:1397:PHE:HZ	1.84	0.42
1:A:1118:LEU:HD23	1:A:1146:LYS:HZ2	1.83	0.42
1:A:1131:MET:C	1:A:1133:LYS:H	2.26	0.42
1:A:1203:PRO:HB2	1:A:1230:ALA:HB1	2.00	0.42
1:A:1238:GLU:HA	1:A:1264:CYS:O	2.19	0.42
1:A:1313:PHE:HD2	1:A:1314:PHE:CE1	2.37	0.42
1:A:1381:HIS:CB	1:A:1382:PRO:HD3	2.47	0.42
1:A:54:ASN:HB3	1:A:55:SER:H	1.58	0.42
1:A:940:ASN:O	1:A:1393:LEU:HD22	2.19	0.42
1:A:958:SER:O	1:A:962:ARG:HG2	2.19	0.42
1:A:1057:LYS:HA	1:A:1081:SER:O	2.19	0.42
1:A:232:SER:OG	1:A:233:SER:N	2.51	0.42
1:A:1308:GLU:HA	1:A:1311:ARG:NH1	2.35	0.42
1:A:1321:PRO:CA	1:A:1351:SER:OG	2.66	0.42
1:A:15:ILE:HD13	1:A:121:ARG:HH12	1.83	0.42
1:A:121:ARG:O	1:A:123:GLU:HG2	2.19	0.42
1:A:214:TRP:O	1:A:231:LYS:NZ	2.52	0.42
1:A:504:LEU:HD11	1:A:519:ILE:HA	2.00	0.42
1:A:509:ILE:HG21	1:A:518:ILE:CD1	2.49	0.42
1:A:788:SER:HB3	1:A:832:MET:HE1	2.00	0.42
1:A:1068:ALA:O	1:A:1071:GLU:HB3	2.19	0.42
1:A:1095:PHE:CE2	1:A:1120:VAL:HG13	2.54	0.42
1:A:1327:ASN:CG	1:A:1357:ILE:HB	2.44	0.42
1:A:1388:ILE:HG12	2:C:465:ASN:ND2	2.34	0.42
2:C:440:GLY:HA2	2:C:443:ILE:HD12	2.00	0.42
1:A:144:ARG:HB2	1:A:145:PRO:HD3	2.01	0.42
1:A:1006:VAL:HB	1:A:1034:LEU:HG	2.01	0.42
1:A:1044:ILE:O	1:A:1047:ALA:N	2.52	0.42
1:A:1278:SER:HA	1:A:1281:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:HB2	1:A:188:PHE:CE2	2.54	0.42
1:A:505:SER:O	1:A:551:ASP:HB3	2.19	0.42
1:A:593:LEU:CD2	1:A:594:GLY:O	2.57	0.42
1:A:918:LYS:HG2	1:A:919:VAL:N	2.34	0.42
1:A:995:LYS:HD2	1:A:995:LYS:N	2.34	0.42
1:A:141:ARG:NH2	1:A:205:GLY:HA3	2.34	0.42
1:A:203:SER:OG	1:A:204:LEU:N	2.52	0.42
1:A:462:LEU:O	1:A:463:ASN:ND2	2.42	0.42
1:A:509:ILE:CD1	1:A:518:ILE:CG2	2.49	0.42
1:A:17:TYR:HD2	1:A:48:LYS:HZ3	1.64	0.42
1:A:493:PRO:O	1:A:494:LEU:C	2.62	0.42
1:A:509:ILE:HG23	1:A:518:ILE:HG12	2.01	0.42
1:A:561:GLN:O	1:A:565:THR:HB	2.20	0.42
1:A:1066:SER:O	1:A:1068:ALA:N	2.53	0.42
1:A:1167:LEU:O	1:A:1190:GLY:HA2	2.20	0.42
1:A:1311:ARG:NH2	1:A:1339:GLN:HG3	2.34	0.42
1:A:134:ASN:CG	1:A:135:ILE:N	2.78	0.42
1:A:159:GLU:HA	1:A:162:ARG:CG	2.50	0.42
1:A:242:SER:OG	1:A:243:TYR:N	2.53	0.42
1:A:452:ALA:O	1:A:453:LEU:HD23	2.20	0.42
1:A:943:PRO:HD2	1:A:944:PRO:HD3	2.00	0.42
1:A:971:ILE:HG12	2:C:482:GLN:OE1	2.19	0.42
1:A:1087:THR:O	1:A:1111:LEU:HG	2.20	0.42
1:A:1097:ASN:CG	1:A:1100:LYS:HZ3	2.28	0.42
1:A:212:ASP:O	1:A:216:GLU:HG2	2.20	0.42
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.89	0.42
1:A:611:LEU:HB3	1:A:621:CYS:SG	2.60	0.42
1:A:775:TYR:O	1:A:777:ARG:N	2.53	0.42
1:A:783:LEU:HD23	1:A:783:LEU:HA	1.71	0.42
1:A:1056:THR:O	1:A:1080:GLN:HB2	2.19	0.42
1:A:1361:MET:HB3	1:A:1363:SER:OG	2.20	0.42
1:A:1364:TRP:HB2	1:A:1367:ASP:HB2	2.01	0.42
1:A:437:ASP:HB3	1:A:455:ILE:CD1	2.50	0.41
1:A:482:ARG:NH2	1:A:486:LEU:CD1	2.82	0.41
1:A:584:ASN:HD21	1:A:732:PHE:N	2.17	0.41
1:A:456:PRO:O	1:A:459:PHE:HB2	2.19	0.41
1:A:632:ASN:HA	1:A:635:LEU:CG	2.49	0.41
1:A:695:GLN:HE21	1:A:756:ARG:HH21	1.68	0.41
1:A:970:ILE:HD12	2:C:479:VAL:HG11	2.02	0.41
1:A:1001:LYS:HG2	1:A:1029:SER:OG	2.19	0.41
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:ILE:O	1:A:975:GLU:HG3	2.21	0.41
1:A:1095:PHE:CD1	1:A:1098:LEU:HD22	2.55	0.41
1:A:1353:LEU:HB2	1:A:1378:LYS:NZ	2.35	0.41
1:A:121:ARG:O	1:A:123:GLU:N	2.53	0.41
1:A:576:CYS:O	1:A:577:LEU:HD12	2.21	0.41
2:C:450:SER:HB3	2:C:453:ARG:H	1.86	0.41
1:A:104:LEU:HD13	1:A:116:ARG:CZ	2.50	0.41
1:A:135:ILE:CB	1:A:492:CYS:HA	2.27	0.41
1:A:139:ASP:O	1:A:142:VAL:N	2.42	0.41
1:A:1106:GLU:OE1	1:A:1133:LYS:HB3	2.21	0.41
1:A:1310:TYR:HA	1:A:1313:PHE:HB3	2.02	0.41
1:A:1367:ASP:HA	1:A:1370:ASP:HB2	2.03	0.41
1:A:1368:GLU:O	1:A:1371:MET:HB2	2.20	0.41
1:A:113:PRO:O	1:A:114:ILE:C	2.64	0.41
1:A:245:GLY:HA3	1:A:463:ASN:ND2	2.25	0.41
1:A:535:LEU:O	1:A:539:ILE:HG13	2.21	0.41
1:A:909:GLU:HG3	1:A:998:LYS:HE2	2.02	0.41
1:A:922:ASN:HD21	1:A:925:LYS:HE3	1.85	0.41
1:A:944:PRO:HB2	1:A:1395:VAL:HA	2.03	0.41
1:A:1118:LEU:HD12	1:A:1119:SER:N	2.35	0.41
1:A:212:ASP:H	1:A:215:LYS:HD3	1.85	0.41
1:A:532:GLU:O	1:A:536:SER:N	2.54	0.41
1:A:552:ASP:CG	1:A:553:TYR:N	2.78	0.41
1:A:828:ASN:CG	1:A:832:MET:HE3	2.46	0.41
1:A:909:GLU:HG2	1:A:909:GLU:O	2.20	0.41
1:A:962:ARG:O	1:A:963:ASN:C	2.63	0.41
1:A:1135:SER:CB	1:A:1163:LYS:HB2	2.51	0.41
1:A:1292:GLN:HA	1:A:1322:ASN:HD22	1.84	0.41
1:A:217:HIS:CD2	1:A:227:LEU:HD22	2.53	0.41
1:A:635:LEU:CG	1:A:636:GLN:H	2.33	0.41
1:A:813:LEU:HD23	1:A:813:LEU:HA	1.80	0.41
1:A:893:THR:HA	1:A:914:LEU:O	2.20	0.41
1:A:896:LEU:HD11	1:A:1002:LEU:HD11	2.03	0.41
1:A:1088:ASN:CB	1:A:1114:LYS:HZ2	2.29	0.41
1:A:1247:GLY:HA2	1:A:1249:HIS:CD2	2.56	0.41
3:A:1501:ATP:O1B	3:A:1501:ATP:O1A	2.39	0.41
1:A:64:LEU:HA	1:A:64:LEU:HD23	1.83	0.41
1:A:100:CYS:CB	1:A:117:HIS:HE2	2.34	0.41
1:A:477:THR:O	1:A:481:LYS:HG3	2.20	0.41
1:A:515:LEU:H	1:A:518:ILE:HG13	1.86	0.41
1:A:733:THR:HG22	1:A:734:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:MET:HE1	1:A:849:TRP:CZ3	2.55	0.41
1:A:832:MET:O	1:A:833:LYS:C	2.62	0.41
1:A:902:GLN:OE1	1:A:905:ARG:HA	2.21	0.41
1:A:949:GLU:OE1	1:A:1365:LEU:N	2.52	0.41
1:A:1066:SER:C	1:A:1068:ALA:N	2.78	0.41
1:A:1118:LEU:HD23	1:A:1146:LYS:NZ	2.36	0.41
1:A:1151:ILE:HG12	1:A:1175:ALA:HB1	2.02	0.41
1:A:1163:LYS:HB3	1:A:1187:GLU:OE1	2.21	0.41
1:A:1397:PHE:HB3	1:A:1400:VAL:HB	2.02	0.41
2:C:456:ASP:O	2:C:460:ALA:N	2.27	0.41
2:C:486:VAL:HB	2:C:487:PRO:HD3	2.03	0.41
1:A:32:PHE:HA	1:A:980:ARG:NH2	2.35	0.41
1:A:137:LYS:HE3	1:A:140:ILE:CG1	2.51	0.41
1:A:245:GLY:HA2	1:A:463:ASN:ND2	2.36	0.41
1:A:414:ALA:HA	1:A:417:ARG:HB2	2.03	0.41
1:A:729:MET:O	1:A:744:LEU:HB2	2.21	0.41
1:A:866:ARG:HG2	1:A:901:LEU:HD21	2.02	0.41
1:A:866:ARG:CG	1:A:901:LEU:HD21	2.51	0.41
1:A:1055:VAL:O	1:A:1056:THR:OG1	2.38	0.41
1:A:1189:SER:OG	1:A:1214:LYS:HG2	2.21	0.41
1:A:1264:CYS:HA	1:A:1293:LYS:CE	2.48	0.41
1:A:76:TRP:HB2	1:A:81:MET:HE2	2.02	0.40
1:A:467:CYS:HB2	1:A:597:LEU:N	2.23	0.40
1:A:646:ALA:HA	1:A:649:CYS:HB3	2.02	0.40
1:A:673:GLN:O	1:A:677:LEU:HG	2.20	0.40
1:A:914:LEU:HG	1:A:1001:LYS:HD2	2.03	0.40
1:A:1247:GLY:C	1:A:1249:HIS:H	2.29	0.40
1:A:1254:LEU:C	1:A:1256:VAL:N	2.79	0.40
1:A:1301:MET:CE	1:A:1304:LYS:H	2.34	0.40
1:A:11:ARG:HG2	1:A:12:ILE:O	2.21	0.40
1:A:408:ARG:HA	1:A:411:TYR:HD2	1.85	0.40
1:A:732:PHE:HE1	1:A:741:TYR:CE1	2.38	0.40
1:A:978:ARG:NH2	2:C:435:LYS:HE3	2.35	0.40
1:A:1016:LEU:O	1:A:1020:LEU:HG	2.21	0.40
1:A:1020:LEU:HA	1:A:1023:VAL:CG2	2.52	0.40
1:A:1048:LEU:HA	1:A:1048:LEU:HD23	1.88	0.40
1:A:1279:VAL:O	1:A:1282:ILE:HB	2.21	0.40
1:A:180:VAL:HA	1:A:183:ALA:HB3	2.02	0.40
1:A:472:THR:C	1:A:474:SER:N	2.78	0.40
1:A:1150:PHE:HA	1:A:1153:ASN:ND2	2.37	0.40
1:A:1199:VAL:HG23	1:A:1200:ASN:CG	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:SER:OG	1:A:1352:ARG:N	2.54	0.40
1:A:147:LYS:HB3	1:A:150:ARG:HH22	1.86	0.40
1:A:408:ARG:HA	1:A:411:TYR:CD2	2.56	0.40
1:A:445:ILE:H	1:A:595:THR:HG22	1.86	0.40
1:A:708:PHE:HB2	1:A:741:TYR:CE2	2.56	0.40
1:A:1071:GLU:O	1:A:1074:LEU:N	2.55	0.40
1:A:1161:HIS:C	1:A:1185:GLU:HB2	2.47	0.40
1:A:1381:HIS:CD2	1:A:1382:PRO:HD3	2.56	0.40
1:A:169:TRP:HE1	1:A:193:ASP:HB2	1.87	0.40
1:A:701:LEU:HD23	1:A:789:PHE:CD1	2.56	0.40
1:A:1064:GLU:OE1	1:A:1089:GLN:HG3	2.21	0.40
1:A:1098:LEU:HD12	1:A:1102:LEU:HD12	2.04	0.40
1:A:1144:LEU:O	1:A:1148:VAL:HG23	2.20	0.40
1:A:1198:PHE:O	1:A:1203:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1234/1403 (88%)	1016 (82%)	204 (16%)	14 (1%)	11	45
2	C	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
All	All	1307/1478 (88%)	1082 (83%)	211 (16%)	14 (1%)	14	45

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	PRO
1	A	1055	VAL
1	A	601	GLU
1	A	740	VAL

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Mol	Chain	Res	Type
1	A	874	GLU
1	A	948	GLU
1	A	788	SER
1	A	619	ILE
1	A	135	ILE
1	A	946	ILE
1	A	983	PRO
1	A	1159	VAL
1	A	15	ILE
1	A	468	VAL

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	1118/1259 (89%)	1116 (100%)	2 (0%)	87	85
2	C	56/56 (100%)	56 (100%)	0	100	100
All	All	1174/1315 (89%)	1172 (100%)	2 (0%)	85	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	A	553	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	43	HIS
1	A	88	HIS
1	A	228	GLN
1	A	406	GLN
1	A	418	HIS

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Mol	Chain	Res	Type
1	A	463	ASN
1	A	499	GLN
1	A	582	HIS
1	A	584	ASN
1	A	824	ASN
1	A	922	ASN
1	A	956	HIS
1	A	973	ASN
1	A	1089	GLN
1	A	1099	HIS
1	A	1130	HIS
1	A	1152	GLN
1	A	1161	HIS
1	A	1200	ASN
1	A	1236	ASN
1	A	1322	ASN
1	A	1337	GLN
1	A	1339	GLN
1	A	1375	ASN
2	C	465	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
3	ATP	A	1501	-	32,33,33	1.32	5 (15%)	48,52,52	1.77	8 (16%)

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
3	ATP	A	1501	-	-	5/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	ATP	C5-C4	4.56	1.47	1.39
3	A	1501	ATP	C5-N7	-2.85	1.33	1.39
3	A	1501	ATP	C5-C6	2.35	1.47	1.41
3	A	1501	ATP	C4-N9	-2.20	1.33	1.37
3	A	1501	ATP	C8-N7	2.08	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	ATP	C5-C4-N3	-5.82	118.70	126.72
3	A	1501	ATP	N3-C4-N9	4.55	134.91	127.17
3	A	1501	ATP	C4-C5-N7	-3.42	106.67	110.58
3	A	1501	ATP	C2-N3-C4	3.41	120.17	111.83
3	A	1501	ATP	N3-C2-N1	-2.93	124.15	128.58
3	A	1501	ATP	C3'-C2'-C1'	2.67	106.51	101.46
3	A	1501	ATP	C5-N7-C8	2.37	107.18	103.45
3	A	1501	ATP	C4-N9-C8	2.31	108.17	105.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	ATP	C5'-O5'-PA-O1A
3	A	1501	ATP	C5'-O5'-PA-O2A

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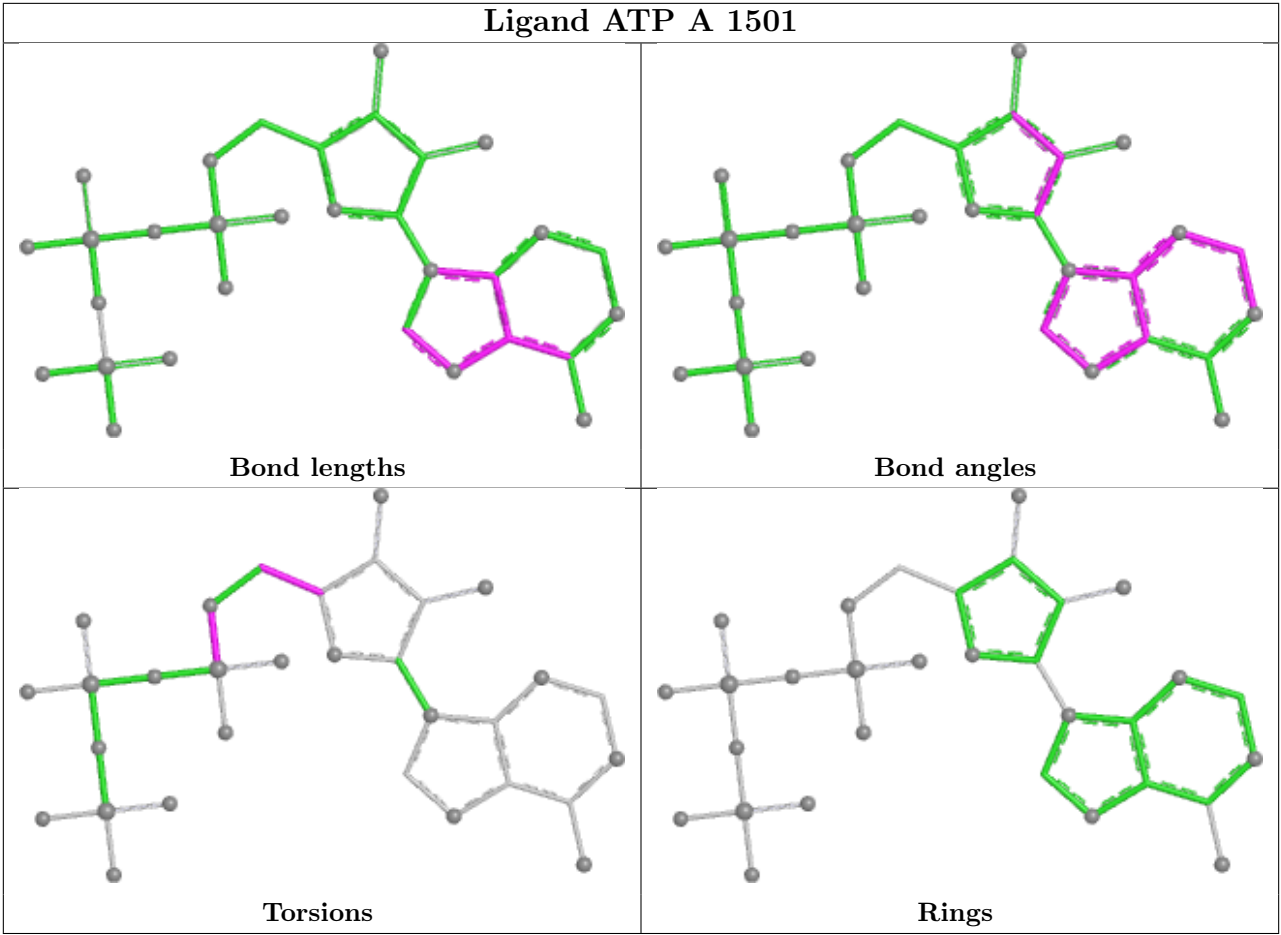
Mol	Chain	Res	Type	Atoms
3	A	1501	ATP	C5'-O5'-PA-O3A
3	A	1501	ATP	O4'-C4'-C5'-O5'
3	A	1501	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	ATP	9	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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	76:TRP	C	77:THR	N	1.19

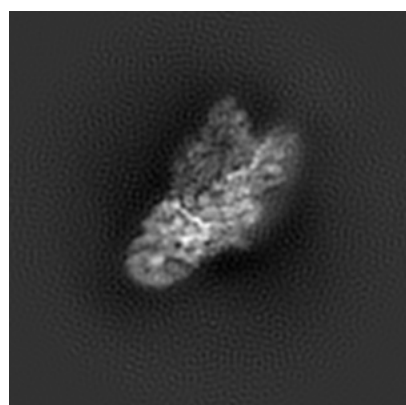
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6845. These allow visual inspection of the internal detail of the map and identification of artifacts.

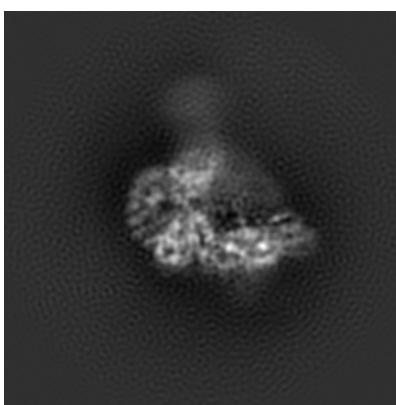
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

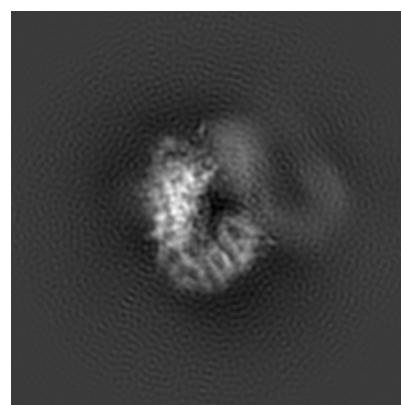
6.1.1 Primary map



X



Y

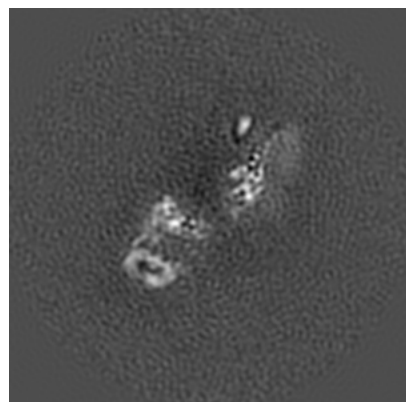


Z

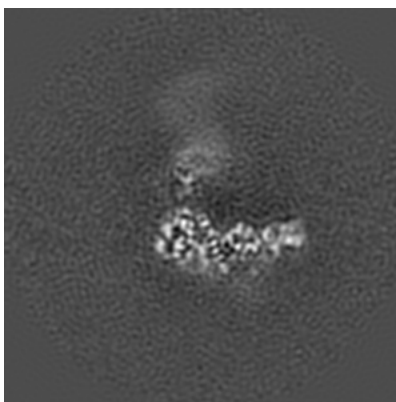
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

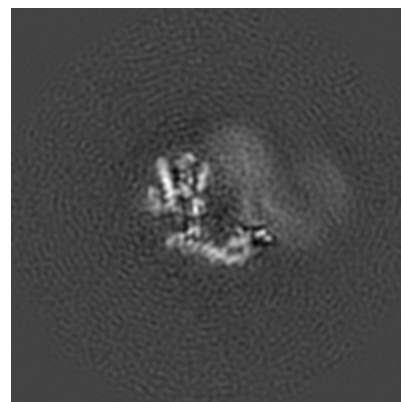
6.2.1 Primary map



X Index: 100



Y Index: 100

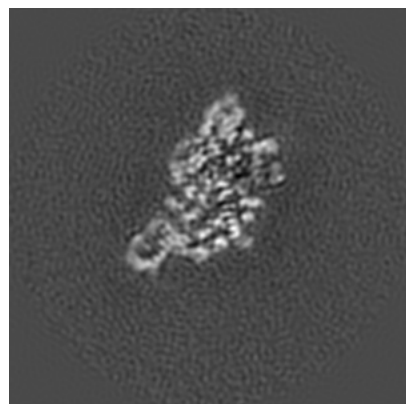


Z Index: 100

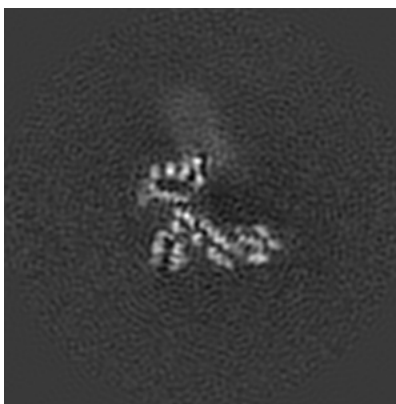
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

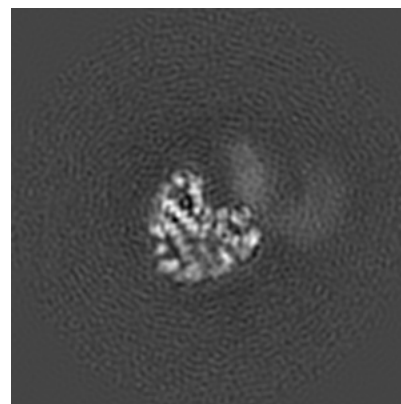
6.3.1 Primary map



X Index: 84



Y Index: 90

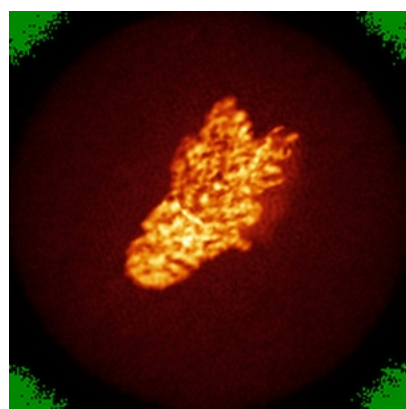


Z Index: 86

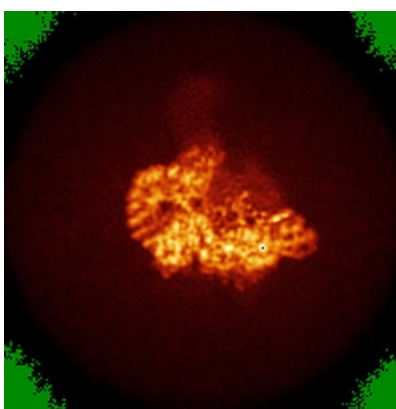
The images above show the largest variance slices of the map in three orthogonal directions.

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

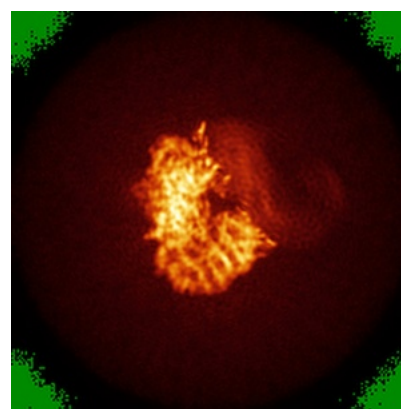
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0252. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

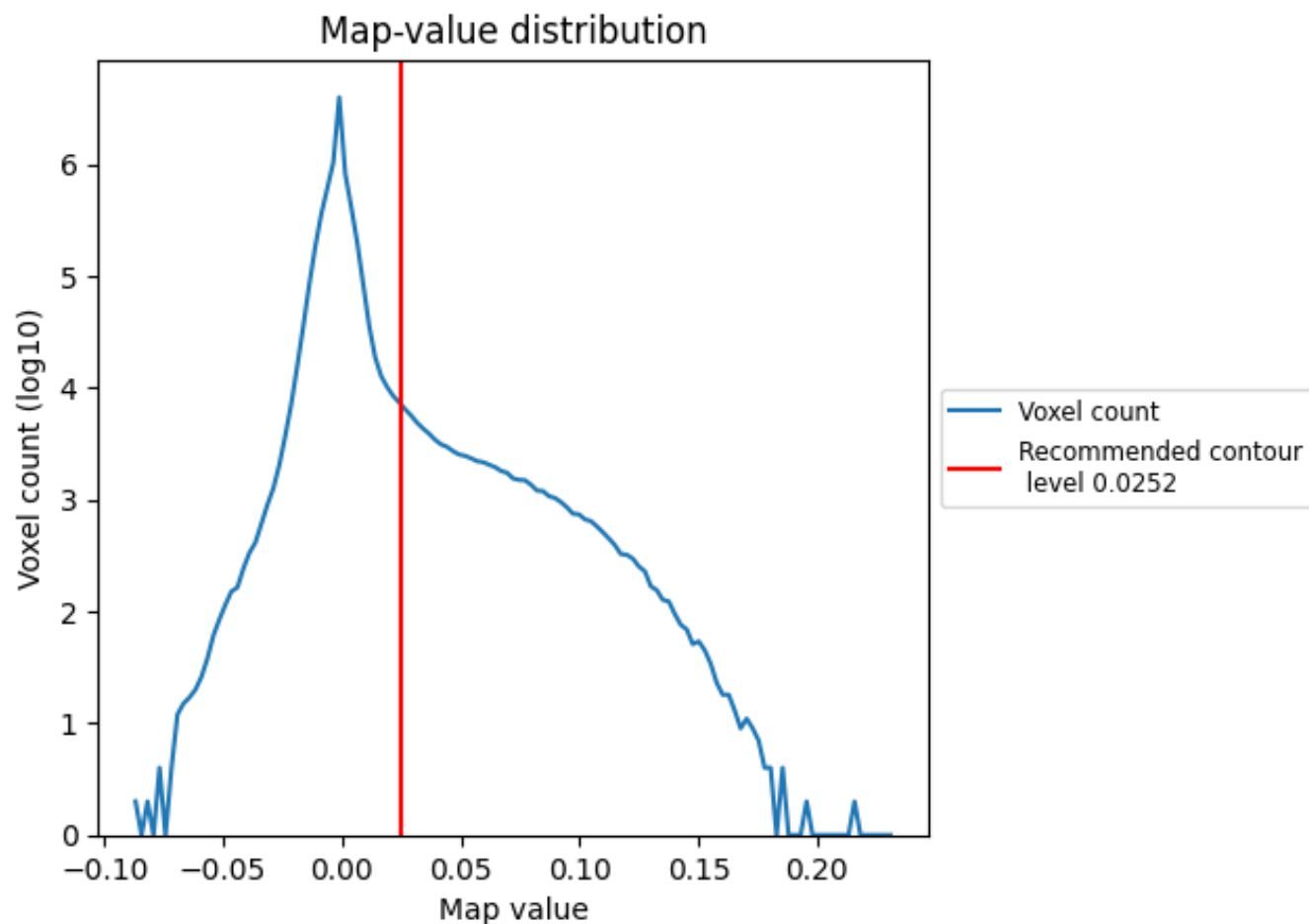
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

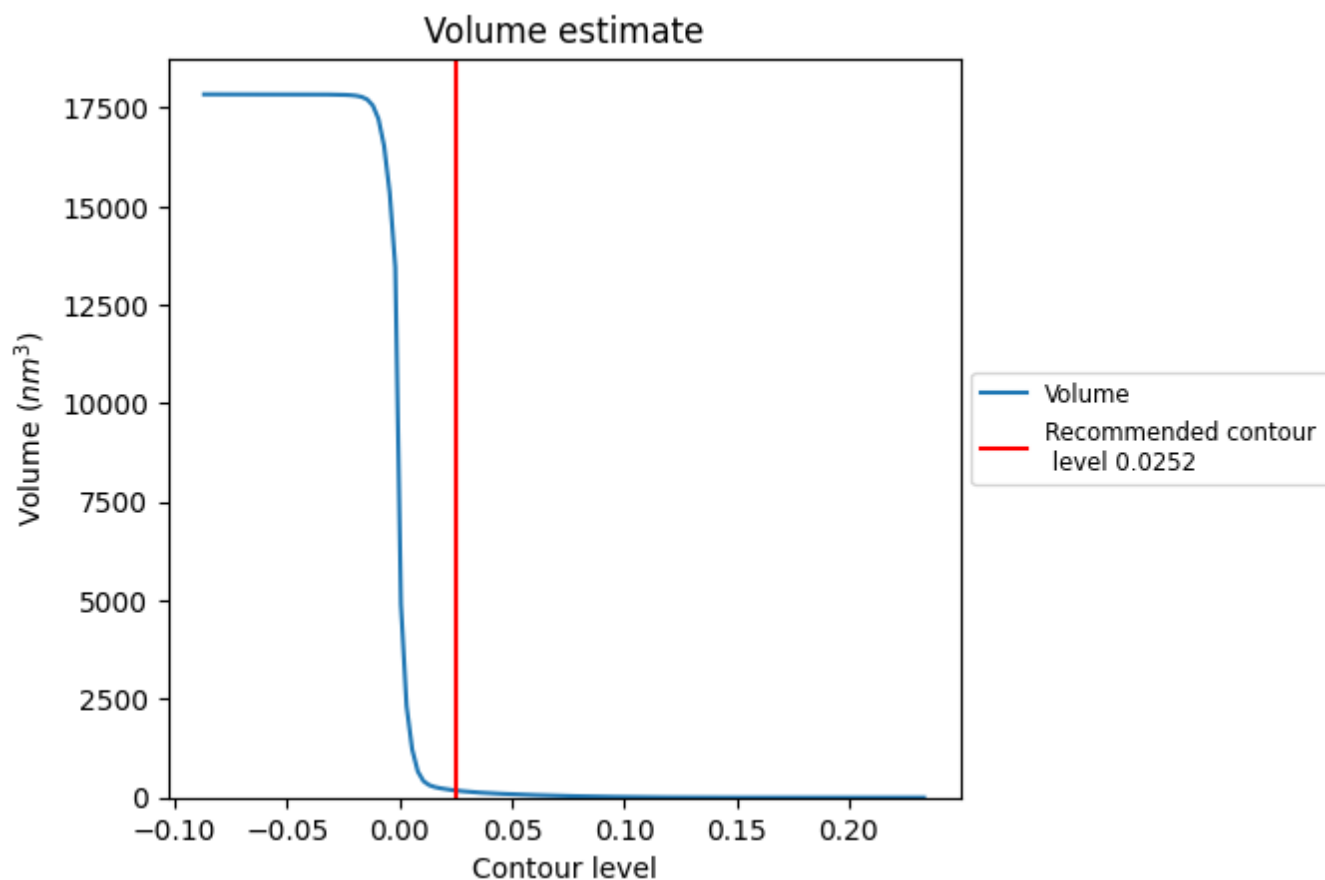
This section contains the results of statistical analysis of the map.

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.

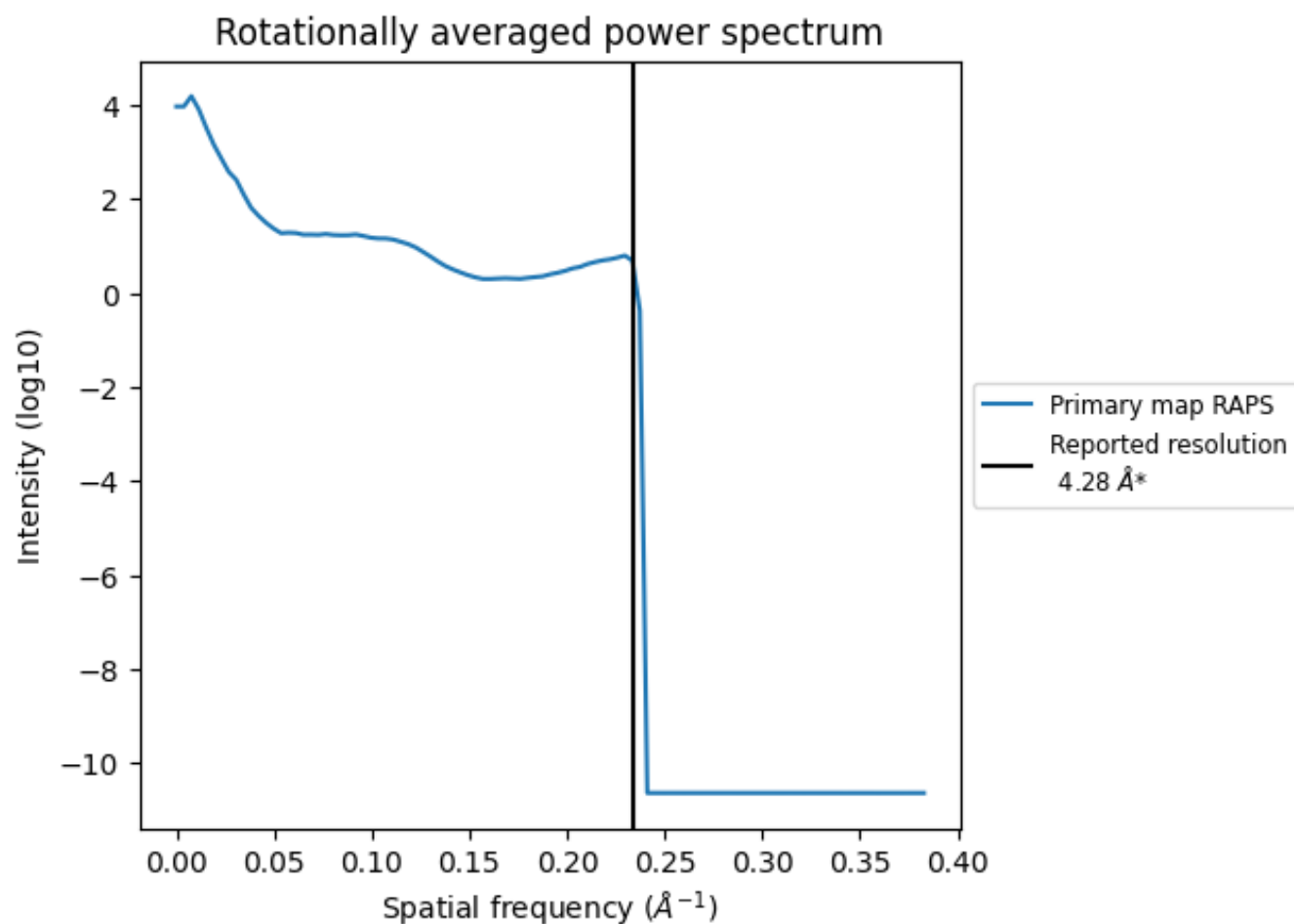
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm^3 ; this corresponds to an approximate mass of 162 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 ⓘ

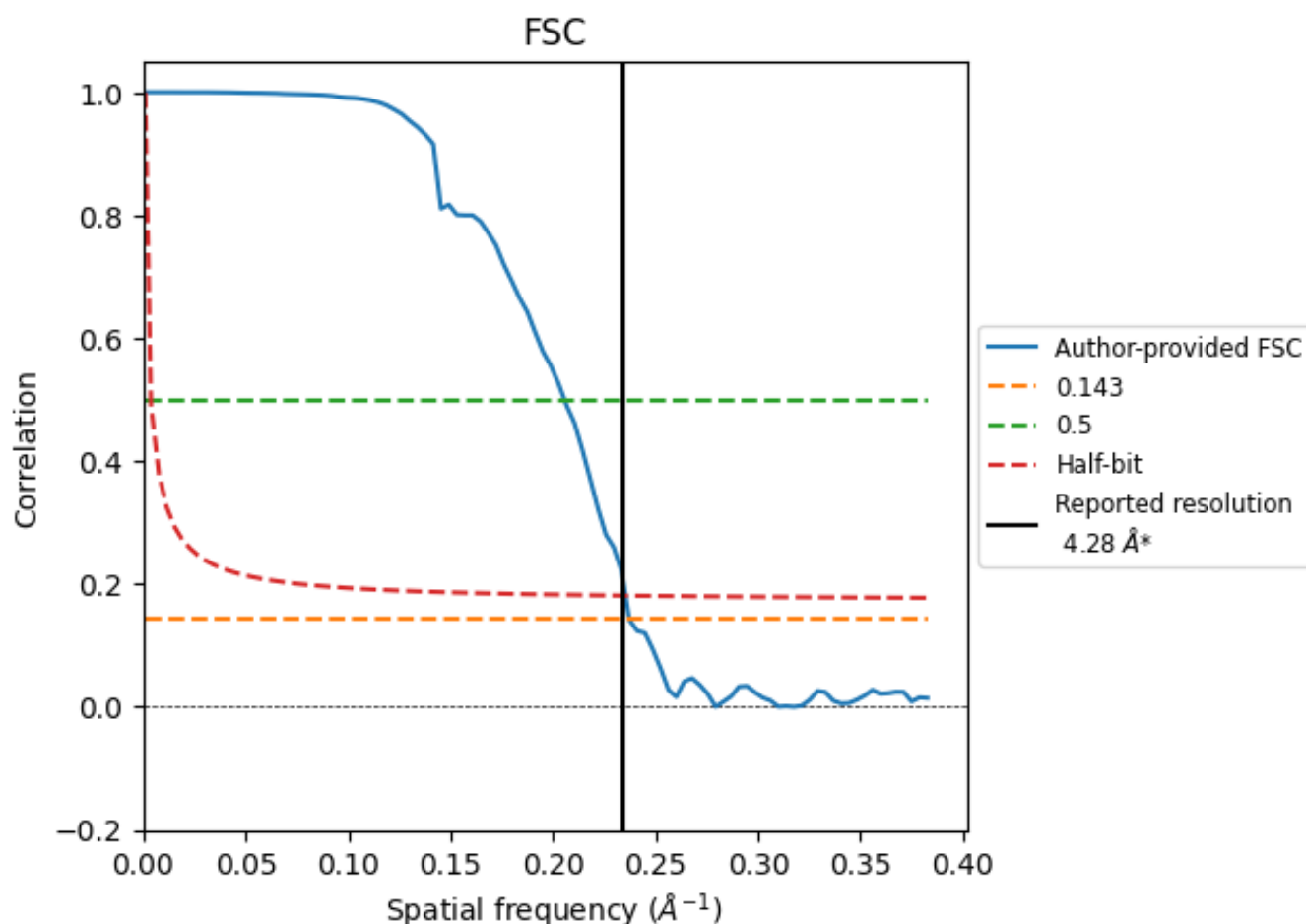


*Reported resolution corresponds to spatial frequency of 0.234 $\text{\AA}^{-1}$

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 0.234 Å⁻¹

8.2 Resolution estimates [i](#)

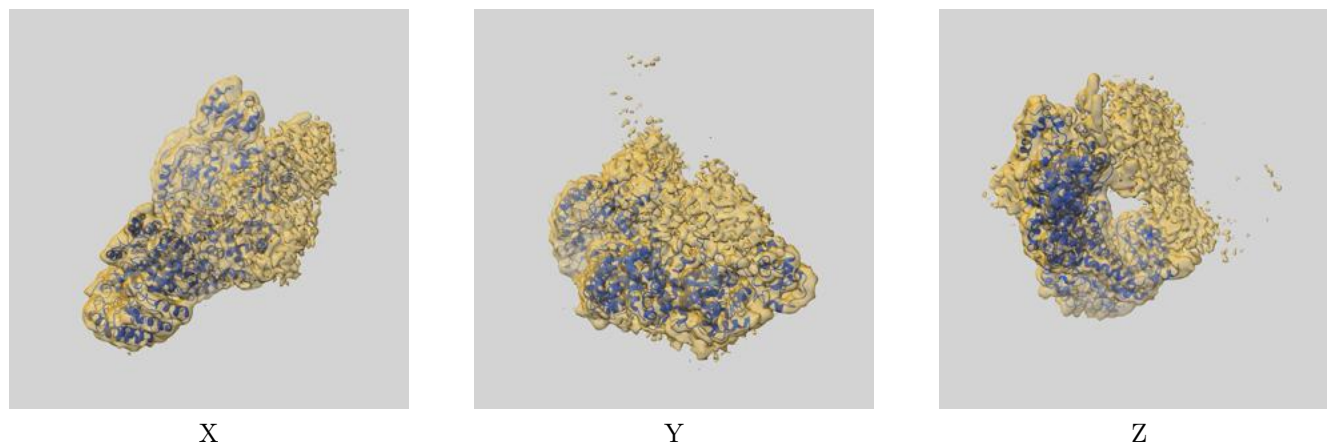
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.28	-	-
Author-provided FSC curve	4.22	4.87	4.25
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

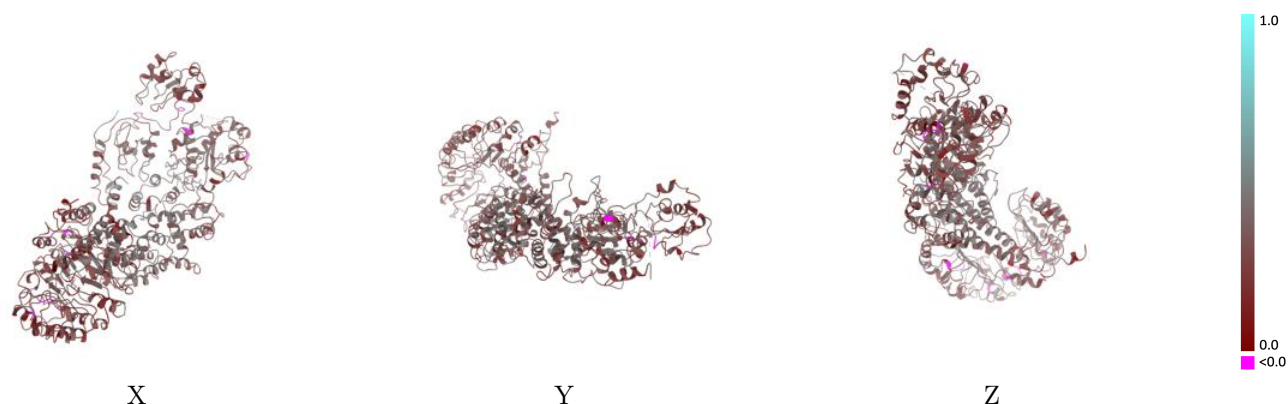
This section contains information regarding the fit between EMDB map EMD-6845 and PDB model 5YUD. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0252 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



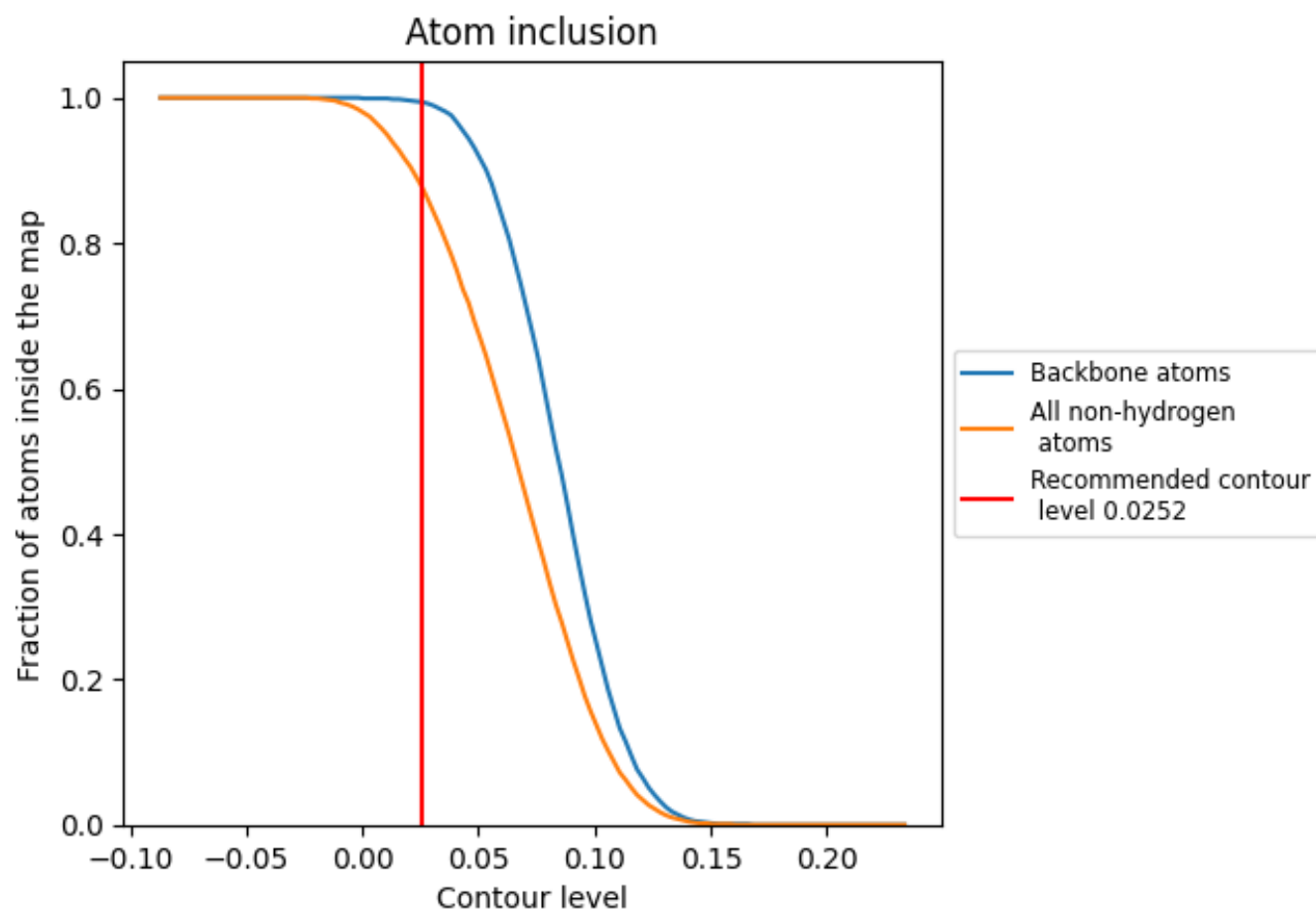
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.0252).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (0.0252) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.3130
A	0.8800	0.3120
C	0.8800	0.3320

