



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:00 PM UTC

PDB ID : 9ZIS / pdb_00009zis
EMDB ID : EMD-74281
Title : C. elegans PEZO-1 Isoform G
Authors : Bell, B.; Baker, M.L.; Vasquez, V.
Deposited on : 2025-12-04
Resolution : 3.50 Å(reported)
Based on initial model : .

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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

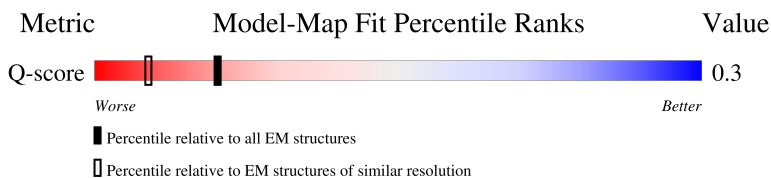
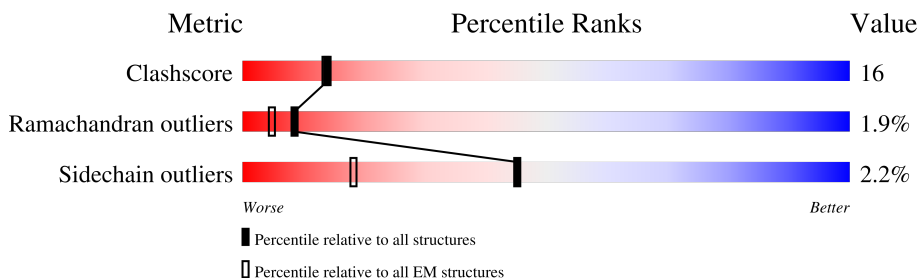
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	2442	
1	B	2442	
1	C	2442	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 44505 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.

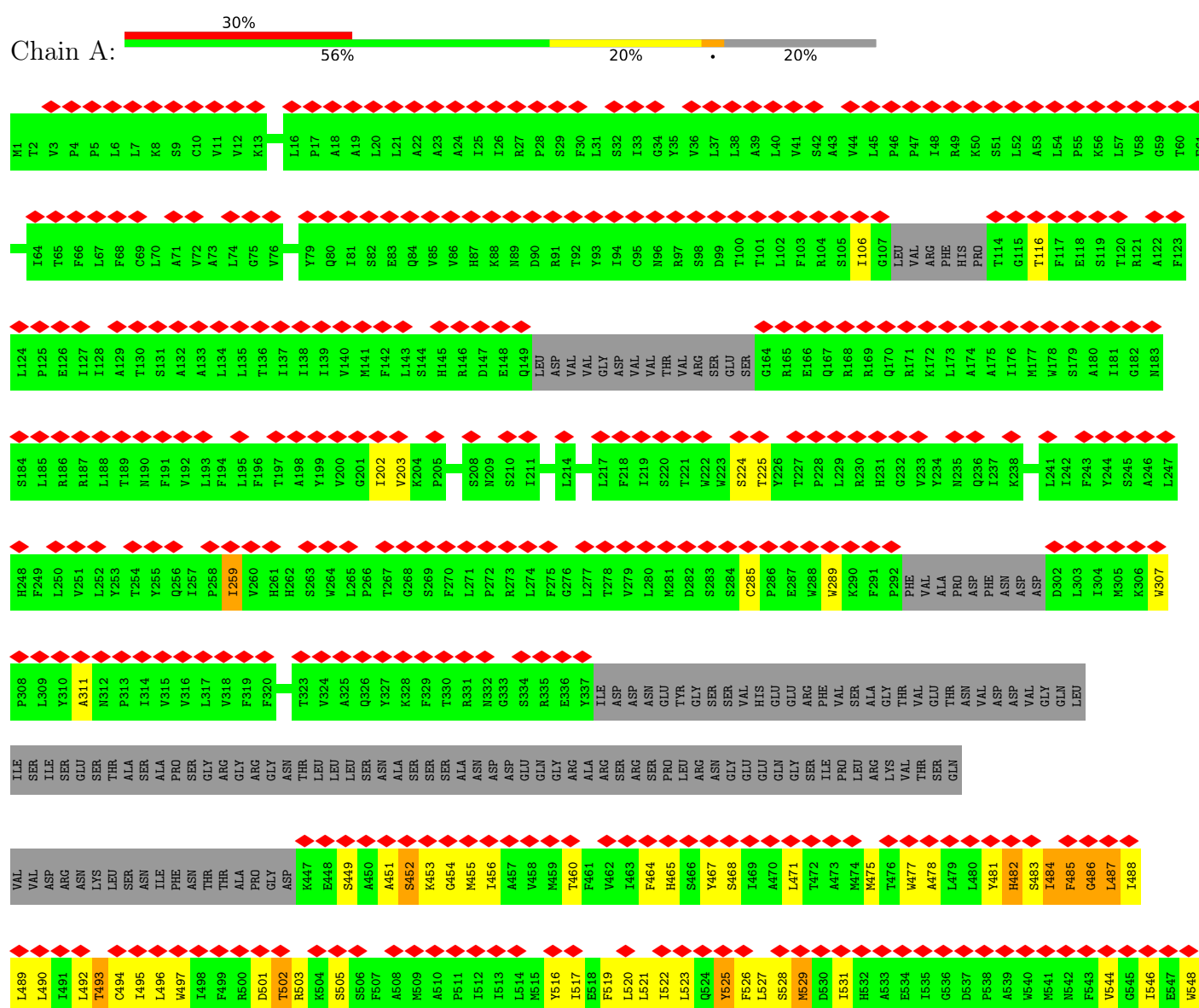
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1944	Total	C	N	O	S	0	0
			14835	9697	2470	2589	79		
1	B	1944	Total	C	N	O	S	0	0
			14835	9697	2470	2589	79		
1	C	1944	Total	C	N	O	S	0	0
			14835	9697	2470	2589	79		

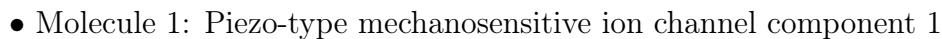
3 Residue-property plots

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: Piezo-type mechanosensitive ion channel component 1



ARG	R1367	R1368	T1369	E1370	G1371	I1372	R1373	E1374	Y1375	Q1376	ALA	Q1377	THR	Q1378	ALA	Q1379	I1380	E1381	R1382	G1383	LEU	A1384	A1385	E1386	R1387	D1388	F1389	E1390	P1391	V1392	T1393	Y1394	G1395	H1396	R1399	M1405	D1409	N1412	D1413	D1414	L1415	V1416	E1417	PRO	VAL	ASP	VAL	ASP	PRO	GLY	PHE	VAL	VAL	PRO	GLU	GLU	VAL	ASP	PRO	GLY	ASP	GLY	GLU
	V1293	E1294	K1295	K1296	E1297	N1298	N1299	I1300	F1301	F1302	D1303	V1304	I1305	A1306	L1307	S1308	V1311	I1314	R1315	F1316	H1317	H1318	W1319	W1320	Y1321	F1322	Q1323	H1324	C1325	M1326	V1327	I1328	Y1329	R1330	S1331	E1332	V1333	I1334	L1335	A1336	N1337	R1338	G1339	L1342	K1343	N1344	Q1345	L1346	I1347	E1348	K1349	L1350	M1351	K1352	ALA	ALA	TYR	ASP					
	H1219	T1220	L1221	W1224	M1225	A1226	L1227	L1228	L1232	I1235	T1236	M1237	K1238	V1239	C1240	L1241	Q1242	I1243	F1244	F1247	F1248	L1249	S1250	W1251	F1252	Q1253	Q1254	S1255	G1256	G1257	W1258	K1259	K1260	T1261	L1262	G1263	I1264	V1265	R1266	Q1267	L1268	F1269	S1270	I1271	T1272	C1273	H1279	V1280	L1281	K1282	E1283	L1284	C1291	A1292									
	PRO	E1145	Y1149	D1150	F1151	I1152	T1153	T1154	K1155	K1156	S1157	Y1158	V1159	D1160	Y1161	F1162	K1163	S1164	H1168	L1175	M1176	S1177	T1178	L1179	A1180	A1181	G1182	I1183	A1184	G1185	T1186	S1187	A1190	L1191	G1192	Y1193	I1194	I1195	F1196	T1197	S1203	G1204	L1207	Y1208	V1209	M1210	N1211	S1212	T1213	L1214	R1215	S1216	F1217	E1218									
	I989	Q990	F991	L992	I993	D994	Y995	G996	F997	Y998	K999	F1000	G1001	L1002	T1005	M1006	I1007	A1008	I1009	G1010	I1013	R1016	M1017	L1018	A1019	L1020	A1021	A1022	I1023	Q1024	S961	L962	G963	L964	P965	E966	S967	M968	R969	A970	K971	Y972	F973	F976	H977	H978	H979	H980	F981	D982	R983	S984	L985	L1056	F1059								
	GLU	GLY	THR	GLU	PRO	ILE	TYR	MET	LEU	PHE	G937	V938	I939	V940	S941	I942	I943	A944	A946	F947	S948	S949	I950	V951	N952	R954	Q955	R956	H957	A960	S961	L962	G963	L964	P965	E966	S967	M968	R969	A970	K971	Y972	F973	F976	H977	H978	H979	H980	F981	D982	R983	S984	L985	L1056	F1059								
	P864	S865	A866	D867	D868	G869	I870	F871	F874	M875	C876	A877	Y878	L879	V882	S885	K886	M887	ILE	TYR	GLN	LEU	ASP	ILE	VAL	PRO	GLU	LEU	SER	GLN	ILE	ASP	ARG	VAL	GLY	ALA	ASP	ASN	CYS	SER	HIS	GLY	ASN	ILE	SER	MET	PRO	GLU	PHE	GLY	LYS	LYS	GLU	VAL									
	GLY	THR	GLN	ARG	ALA	HIS	ALA	ALA	ASP	THR	L807	V808	K809	H812	K813	L814	T818	I819	E820	L821	L822	M823	N824	F825	F826	E827	V828	H829	I830	S831	K832	I833	V834	F835	V836	I837	I838	A839	I840	F841	A848	L849	Y850	I851	P852	L853	V854	L857	S858	L859	A860	I861	C862	L863									
	V731	D732	F733	R734	A735	I736	G737	E738	S739	G740	A741	L742	F743	L744	Q745	L746	L747	A748	F749	I750	A751	L752	F753	V754	V755	T756	Q759	L760	I699	I700	A701	L702	Y703	I704	Y705	Q706	F707	W708	ARG	GLU	ALA	GLN	S711	F653	A654	P655	N656	F657	Y658	N659	I660	L661	S719	L720	S721	Q722	E723	W724	A727	I728	G729	L730	
	VAL	ALA	VAL	ALA	LYS	PHE	Q616	D617	P618	K619	S620	R621	K622	F623	A624	A625	F626	V627	E628	Y629	L630	S631	M632	K633	V634	S635	V636	Y637	F638	I639	F640	V641	V642	S643	V644	V645	L646	L647	V648	V649	S650	T651	C652	F653	A654	P655	N656	F657	Y658	N659	I660	L661	S719	L720	S721	Q722	E723	W724	A727	I728	G729	L730	
	T549	T550	L551	P552	V553	H554	A555	V556	I557	I558	L559	C560	V561	Q562	T563	L564	L565	T566	L567	P568	V569	F570	L571	L572	L573	R574	R577	R578	E579	K580	F581	Y582	E583	S584	LEU	SER	ASP	TYR	GLU	ARG	GLN	ARG	ARG	ILE	ASN	ASN	TYR	GLY	THR	PHE	GLY	ALA	SER	LYS	THR	GLY	ALA	GLY	GLY				



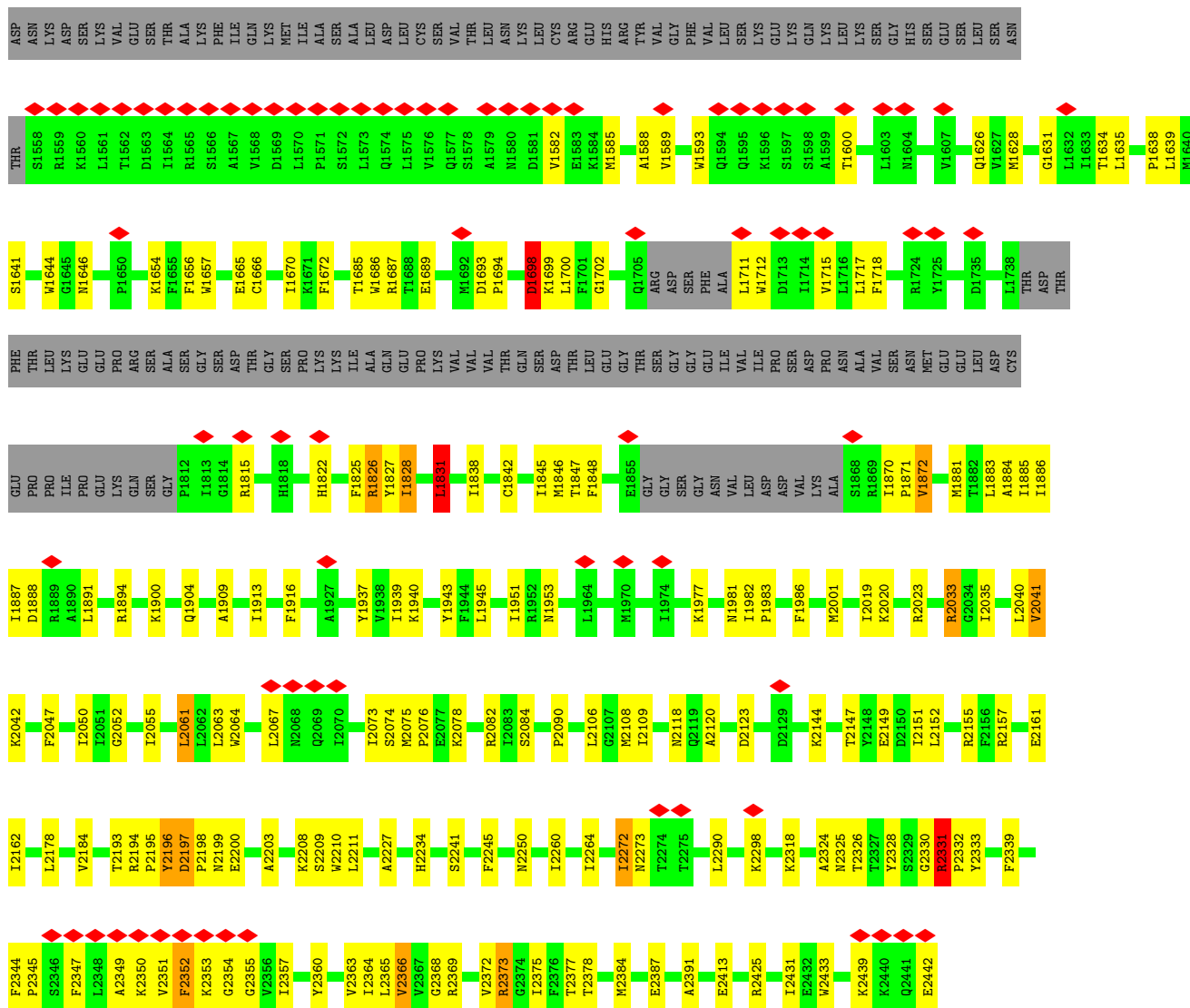
Frequency	Percentage
30%	30%
57%	57%
20%	20%
20%	20%







ASP	T1369	E1294	Y1149	L1064	L992	GLU	A867	GLY	R734	L873	ALA	P552
PRO	E1295	T1295	D1150	P1065	I993	PRO	D868	ARG	A735	K674	LYS	V553
GLY	A1371	K1296	F1151	P1066	I994	ILE	G869	ALA	I736	E875	PHE	H554
ILE	E1297	E1297	I1152	I1070	D994	MET	T870	HIS	G737	S676		A555
MET	E1374	E1298	D1153	E1071	Y995	LEU	F871	ALA	E738	P677		V556
TYR	R1375	N1299	T1154	E1072	G996	PHE	F871	GLY	S739	R678		I557
ALA	Y1376	I1300	K1155	P1073	Y998	G837	F874	ASP	G740	L879		I558
ALA	Q1377	G1301	K1156	W1074	K999	THR	M875	THR	G741	Y880		L559
THR	K1378	F1302	Y1158	W1077	G1001		M875	L807	L742	R681		C560
ALA	Q1379	D1303	V1159	I1078	F1002		G876	V808	F743	K682		V561
HIS	I1380	V1304	D1160	P1078	L1002		A877	K909	L744	G882		Q562
ASP	I1381	I1305	T1161	S1080	T1005		Y878	H812	L745	L883		T563
LEU	R1382	A1306	F1162	S1081	M1006		L879	K813	Q745	A684		L564
ASP	G1383	L1307	K1163	Y1081	I1007		V882	L814	L746	Y685		L565
LEU	A1384	L1308	S1164	S1082	A1008				L747	A686		T566
ALA	A1385	S1308	S1164	Y1083	A1008				L748	P687		L567
LYS	E1386			D1083	G1010				P749	W688		L567
THR	R1387	V1311	H1168	D1084	F947		S885	T818	I750	L689		P568
VAL	D1388				Q948		R886	I819	I751	T690		V569
GLN	F1388				S949		M887	E820	A751	L830		F570
GLN	F1389				S949			L821	L752	S831		L571
VAL	E1390				V951		ILE	L822	F753	T692		L572
LYS	P1391				T952		TYR	W823	W754	K633		L573
LYS	V1392				Y953		GLN	L824	F755	V634		R574
GLY	T1393				R954		LEU	R824	W756	S635		
ASP	S1319				A1019		ASP	F825		V636		R577
ASP	Y1394				Q955		ILE	F826		Y637		R578
THR	Y1321				R956		VAL	F827		F638		E579
ILE	H1396				H957		GLU	W828		I639		K580
LYS					I1023		LEU	L829		F640		F581
ASP	R1399				Q1024		SER	H829		V641		Y582
PRO	M1326				S961		GLN	I830		V642		E583
ASP	V1327				L962		ILE	S831		S643		S584
SER	E1328				G963		ASP	W832		V644		LEU
ARG	Y1329				L964		ARG	I833		V645		SER
ALA	R1330				V965		VAL	W834		L646		ASP
LEU	S1331				P966		GLY	F835		L647		TYR
ILE	E1332				E966		GLY	I837		V648		GLU
ALA	E1333				S967		ALA	L838		S650		ARG
VAL	I1334				R968		ASN	T838		T651		GLN
SER	L1335				H968		ASN	A839		C652		ARG
GLU	L1336				R969		CYS	T840		F653		ILE
PRO	A1336				A970		SER	F941		A654		ASN
GLU	R1337				R1040		HIS			P655		SER
ALA	R1338				R1041		GLY			N656		TYR
ARG	G1339				W1042		ASN			F657		GLY
VAL	L1342				W1043		ILE			Y658		THR
LYS	K1343				F1044		SER			N659		PHE
PRO	N1344				F1045		MET			I660		GLY
THR	Q1345				Y1046		THR			L661		ALA
GLU	L1346				Y1047		PRO			S719		SER
VAL	L1347				I1046		GLU			L720		LYS
ASP	E1348				Y1049		THR			S721		THR
PRO	K1349				M1050		PHE			Q722		GLY
GLY	E1350				I1051		GLY			E723		ALA
ASP	M1351				I1052		LEU			L665		GLY
THR	K1352				L1056		GLY			W666		VAL
ASP	N1355				F1059		THR			A667		ALA
ARG	R1367				V1062		THR			L668		VAL
LEU	R1368				G1063		THR			N669		VAL
										G729		
										L730		
										V731		
										D732		
										F733		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.545	Depositor
Minimum map value	-0.371	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0561	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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	0.67	32/15190 (0.2%)	0.95	95/20664 (0.5%)
1	B	0.67	32/15190 (0.2%)	0.95	95/20664 (0.5%)
1	C	0.67	32/15190 (0.2%)	0.95	95/20664 (0.5%)
All	All	0.67	96/45570 (0.2%)	0.95	285/61992 (0.5%)

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	14
1	B	0	14
1	C	0	14
All	All	0	42

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1330	ARG	C-O	13.70	1.41	1.24
1	B	1330	ARG	C-O	13.66	1.41	1.24
1	A	1330	ARG	C-O	13.65	1.41	1.24
1	A	1079	PRO	N-CD	-13.56	1.28	1.47
1	C	1079	PRO	N-CD	-13.53	1.28	1.47
1	B	1079	PRO	N-CD	-13.52	1.28	1.47
1	B	2332	PRO	C-O	-12.45	1.08	1.23
1	A	2332	PRO	C-O	-12.38	1.08	1.23
1	C	2332	PRO	C-O	-12.38	1.08	1.23
1	A	1072	TYR	CA-C	11.71	1.70	1.52
1	C	1072	TYR	CA-C	11.70	1.70	1.52
1	B	1072	TYR	CA-C	11.70	1.70	1.52
1	C	1331	SER	C-O	11.33	1.38	1.24
1	A	1331	SER	C-O	11.32	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1331	SER	C-O	11.28	1.38	1.24
1	B	1072	TYR	C-O	11.09	1.38	1.24
1	C	1072	TYR	C-O	11.07	1.38	1.24
1	A	1072	TYR	C-O	11.04	1.38	1.24
1	B	2324	ALA	C-O	-10.65	1.10	1.23
1	A	2324	ALA	C-O	-10.63	1.10	1.23
1	C	2331	ARG	C-O	-10.61	1.12	1.23
1	A	2331	ARG	C-O	-10.58	1.12	1.23
1	B	2331	ARG	C-O	-10.58	1.12	1.23
1	C	2324	ALA	C-O	-10.56	1.11	1.23
1	B	468	SER	CA-C	9.55	1.65	1.52
1	C	468	SER	CA-C	9.54	1.65	1.52
1	A	468	SER	CA-C	9.54	1.65	1.52
1	B	451	ALA	C-O	9.11	1.35	1.24
1	A	451	ALA	C-O	9.09	1.35	1.24
1	C	451	ALA	C-O	9.09	1.35	1.24
1	C	2324	ALA	CA-C	-8.89	1.42	1.52
1	A	2324	ALA	CA-C	-8.87	1.42	1.52
1	B	2324	ALA	CA-C	-8.86	1.42	1.52
1	A	2332	PRO	CA-C	-8.65	1.42	1.52
1	B	2332	PRO	CA-C	-8.62	1.42	1.52
1	C	2332	PRO	CA-C	-8.60	1.42	1.52
1	C	1072	TYR	N-CA	8.23	1.55	1.46
1	A	1072	TYR	N-CA	8.22	1.55	1.46
1	B	1072	TYR	N-CA	8.21	1.55	1.46
1	C	465	HIS	C-O	-7.39	1.15	1.24
1	A	465	HIS	C-O	-7.30	1.15	1.24
1	B	465	HIS	C-O	-7.29	1.15	1.24
1	A	998	TYR	C-O	7.16	1.32	1.24
1	B	998	TYR	C-O	7.16	1.32	1.24
1	C	998	TYR	C-O	7.16	1.32	1.24
1	C	2203	ALA	C-O	-6.80	1.16	1.24
1	B	2203	ALA	C-O	-6.79	1.16	1.24
1	A	2203	ALA	C-O	-6.76	1.16	1.24
1	A	468	SER	N-CA	6.33	1.54	1.46
1	B	468	SER	N-CA	6.32	1.54	1.46
1	C	468	SER	N-CA	6.30	1.54	1.46
1	C	502	THR	CA-C	6.20	1.61	1.52
1	A	502	THR	CA-C	6.18	1.61	1.52
1	B	502	THR	CA-C	6.14	1.60	1.52
1	A	1000	PHE	CA-C	-6.10	1.44	1.52
1	C	1000	PHE	CA-C	-6.10	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1000	PHE	CA-C	-6.10	1.44	1.52
1	C	2332	PRO	CA-CB	-6.10	1.45	1.53
1	A	2332	PRO	CA-CB	-6.07	1.45	1.53
1	B	2332	PRO	CA-CB	-6.04	1.45	1.53
1	B	999	LYS	C-O	5.88	1.30	1.24
1	C	999	LYS	C-O	5.86	1.30	1.24
1	A	999	LYS	C-O	5.83	1.30	1.24
1	C	1826	ARG	N-CA	-5.80	1.38	1.46
1	A	1826	ARG	N-CA	-5.79	1.38	1.46
1	B	493	THR	C-O	-5.78	1.17	1.24
1	A	493	THR	C-O	-5.76	1.17	1.24
1	B	1826	ARG	N-CA	-5.76	1.38	1.46
1	C	493	THR	C-O	-5.74	1.17	1.24
1	B	2331	ARG	CA-C	-5.62	1.44	1.52
1	A	2331	ARG	CA-C	-5.61	1.44	1.52
1	C	1831	LEU	C-O	-5.61	1.17	1.24
1	C	2331	ARG	CA-C	-5.61	1.44	1.52
1	A	1831	LEU	C-O	-5.60	1.17	1.24
1	B	1831	LEU	C-O	-5.60	1.17	1.24
1	C	1002	LEU	C-O	5.58	1.30	1.24
1	B	1078	ILE	CA-C	5.57	1.57	1.52
1	A	1002	LEU	C-O	5.57	1.30	1.24
1	C	1078	ILE	CA-C	5.57	1.57	1.52
1	B	1002	LEU	C-O	5.55	1.30	1.24
1	A	1078	ILE	CA-C	5.53	1.57	1.52
1	A	525	TYR	C-O	5.50	1.30	1.24
1	B	525	TYR	C-O	5.47	1.30	1.24
1	A	2377	THR	CA-C	-5.47	1.46	1.52
1	C	525	TYR	C-O	5.47	1.30	1.24
1	B	2377	THR	CA-C	-5.45	1.46	1.52
1	C	2377	THR	CA-C	-5.43	1.46	1.52
1	B	1334	ILE	C-O	5.40	1.30	1.24
1	C	1334	ILE	C-O	5.39	1.30	1.24
1	A	1334	ILE	C-O	5.37	1.30	1.24
1	C	2199	ASN	N-CA	-5.25	1.40	1.46
1	A	2199	ASN	N-CA	-5.24	1.40	1.46
1	B	2199	ASN	N-CA	-5.24	1.40	1.46
1	A	1071	GLU	C-N	5.06	1.42	1.33
1	B	1071	GLU	C-N	5.05	1.42	1.33
1	C	1071	GLU	C-N	5.01	1.42	1.33

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	HIS	N-CA-CB	19.06	142.70	110.49
1	B	482	HIS	N-CA-CB	19.05	142.68	110.49
1	C	482	HIS	N-CA-CB	19.03	142.66	110.49
1	C	680	TYR	CB-CA-C	-17.87	82.82	110.88
1	A	680	TYR	CB-CA-C	-17.87	82.82	110.88
1	B	680	TYR	CB-CA-C	-17.86	82.84	110.88
1	B	2330	GLY	N-CA-C	17.02	137.04	114.92
1	A	2330	GLY	N-CA-C	16.81	137.07	115.21
1	C	2330	GLY	N-CA-C	16.78	137.03	115.21
1	C	2196	TYR	N-CA-C	13.20	127.31	111.33
1	B	2196	TYR	N-CA-C	13.19	127.29	111.33
1	A	2196	TYR	N-CA-C	13.17	127.27	111.33
1	A	468	SER	N-CA-C	12.53	127.10	111.69
1	C	468	SER	N-CA-C	12.53	127.10	111.69
1	B	468	SER	N-CA-C	12.50	127.07	111.69
1	A	451	ALA	N-CA-C	-11.44	97.62	111.69
1	C	451	ALA	N-CA-C	-11.43	97.63	111.69
1	B	451	ALA	N-CA-C	-11.41	97.66	111.69
1	B	1077	TRP	CA-C-N	10.98	127.16	120.24
1	B	1077	TRP	C-N-CA	10.98	127.16	120.24
1	A	1077	TRP	CA-C-N	10.97	127.15	120.24
1	A	1077	TRP	C-N-CA	10.97	127.15	120.24
1	C	1077	TRP	CA-C-N	10.90	127.11	120.24
1	C	1077	TRP	C-N-CA	10.90	127.11	120.24
1	B	1078	ILE	N-CA-C	10.80	128.27	112.61
1	C	1078	ILE	N-CA-C	10.77	128.23	112.61
1	A	1078	ILE	N-CA-C	10.77	128.22	112.61
1	C	2197	ASP	CA-C-N	10.74	131.56	119.32
1	C	2197	ASP	C-N-CA	10.74	131.56	119.32
1	A	2197	ASP	CA-C-N	10.72	131.54	119.32
1	A	2197	ASP	C-N-CA	10.72	131.54	119.32
1	B	2197	ASP	CA-C-N	10.71	131.53	119.32
1	B	2197	ASP	C-N-CA	10.71	131.53	119.32
1	C	1072	TYR	CA-C-O	10.58	128.28	119.71
1	A	1072	TYR	CA-C-O	10.55	128.25	119.71
1	B	1072	TYR	CA-C-O	10.54	128.25	119.71
1	C	680	TYR	N-CA-CB	10.08	124.62	110.01
1	A	680	TYR	N-CA-CB	10.05	124.58	110.01
1	B	680	TYR	N-CA-CB	10.05	124.59	110.01
1	C	1080	SER	N-CA-C	9.62	124.73	111.74
1	B	1080	SER	N-CA-C	9.62	124.73	111.74
1	A	1080	SER	N-CA-C	9.61	124.71	111.74
1	B	1330	ARG	O-C-N	-9.21	110.35	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1330	ARG	O-C-N	-9.20	110.35	122.59
1	A	1330	ARG	O-C-N	-9.20	110.36	122.59
1	C	1078	ILE	CA-C-N	8.33	130.25	119.84
1	C	1078	ILE	C-N-CA	8.33	130.25	119.84
1	A	1831	LEU	N-CA-C	8.32	128.51	110.80
1	B	1831	LEU	N-CA-C	8.31	128.51	110.80
1	C	1831	LEU	N-CA-C	8.31	128.50	110.80
1	A	1078	ILE	CA-C-N	8.31	130.22	119.84
1	A	1078	ILE	C-N-CA	8.31	130.22	119.84
1	B	1078	ILE	CA-C-N	8.30	130.21	119.84
1	B	1078	ILE	C-N-CA	8.30	130.21	119.84
1	A	1267	GLN	CA-C-O	-8.19	110.12	119.79
1	B	1267	GLN	CA-C-O	-8.19	110.13	119.79
1	C	1329	TYR	O-C-N	-8.18	113.45	122.12
1	A	1329	TYR	O-C-N	-8.17	113.46	122.12
1	C	1267	GLN	CA-C-O	-8.16	110.16	119.79
1	B	1329	TYR	O-C-N	-8.16	113.47	122.12
1	B	482	HIS	N-CA-C	-8.15	93.44	110.80
1	A	482	HIS	N-CA-C	-8.13	93.48	110.80
1	C	482	HIS	N-CA-C	-8.13	93.49	110.80
1	B	678	ARG	N-CA-C	-8.06	102.47	111.82
1	A	678	ARG	N-CA-C	-8.06	102.47	111.82
1	A	1072	TYR	N-CA-C	8.02	124.31	108.59
1	C	1072	TYR	N-CA-C	8.02	124.31	108.59
1	B	1072	TYR	N-CA-C	8.02	124.31	108.59
1	C	678	ARG	N-CA-C	-8.02	102.52	111.82
1	B	2332	PRO	CB-CA-C	-7.93	101.24	111.39
1	A	2332	PRO	CB-CA-C	-7.91	101.26	111.39
1	C	2332	PRO	CB-CA-C	-7.89	101.29	111.39
1	C	493	THR	CA-C-N	7.86	131.85	120.38
1	C	493	THR	C-N-CA	7.86	131.85	120.38
1	A	493	THR	CA-C-N	7.85	131.85	120.38
1	A	493	THR	C-N-CA	7.85	131.85	120.38
1	B	493	THR	CA-C-N	7.84	131.83	120.38
1	B	493	THR	C-N-CA	7.84	131.83	120.38
1	A	451	ALA	O-C-N	7.67	132.21	122.23
1	C	451	ALA	O-C-N	7.64	132.17	122.23
1	B	451	ALA	O-C-N	7.64	132.16	122.23
1	A	1079	PRO	N-CA-C	7.50	127.91	112.47
1	B	1079	PRO	N-CA-C	7.49	127.91	112.47
1	C	1079	PRO	N-CA-C	7.49	127.89	112.47
1	A	1698	ASP	CA-CB-CG	7.30	119.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1698	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	1698	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	998	TYR	CA-C-N	-7.25	110.71	120.79
1	A	998	TYR	C-N-CA	-7.25	110.71	120.79
1	B	998	TYR	CA-C-N	-7.25	110.71	120.79
1	B	998	TYR	C-N-CA	-7.25	110.71	120.79
1	C	998	TYR	CA-C-N	-7.22	110.76	120.79
1	C	998	TYR	C-N-CA	-7.22	110.76	120.79
1	C	1376	TYR	N-CA-CB	7.19	120.81	110.16
1	C	1252	PHE	CA-C-O	-7.18	110.24	120.51
1	B	1376	TYR	N-CA-CB	7.18	120.78	110.16
1	A	1252	PHE	CA-C-O	-7.18	110.25	120.51
1	A	1376	TYR	N-CA-CB	7.17	120.78	110.16
1	B	1252	PHE	CA-C-O	-7.16	110.27	120.51
1	B	456	ILE	N-CA-C	7.11	117.83	110.36
1	A	456	ILE	N-CA-C	7.11	117.82	110.36
1	C	456	ILE	N-CA-C	7.11	117.82	110.36
1	B	2377	THR	N-CA-C	7.01	120.92	109.85
1	A	2377	THR	N-CA-C	7.00	120.90	109.85
1	C	2377	THR	N-CA-C	6.97	120.87	109.85
1	A	1267	GLN	N-CA-C	-6.87	103.57	112.23
1	B	1267	GLN	N-CA-C	-6.87	103.58	112.23
1	C	1071	GLU	CA-C-N	6.86	137.20	122.17
1	C	1071	GLU	C-N-CA	6.86	137.20	122.17
1	A	259	ILE	N-CA-C	6.86	123.61	109.34
1	A	1071	GLU	CA-C-N	6.86	137.19	122.17
1	A	1071	GLU	C-N-CA	6.86	137.19	122.17
1	B	259	ILE	N-CA-C	6.86	123.60	109.34
1	B	1071	GLU	CA-C-N	6.86	137.18	122.17
1	B	1071	GLU	C-N-CA	6.86	137.18	122.17
1	C	259	ILE	N-CA-C	6.86	123.60	109.34
1	C	1267	GLN	N-CA-C	-6.84	103.61	112.23
1	C	2331	ARG	CA-C-N	6.74	126.77	119.89
1	C	2331	ARG	C-N-CA	6.74	126.77	119.89
1	A	2331	ARG	CA-C-N	6.72	126.75	119.89
1	A	2331	ARG	C-N-CA	6.72	126.75	119.89
1	A	1339	GLY	CA-C-N	-6.71	107.90	121.18
1	A	1339	GLY	C-N-CA	-6.71	107.90	121.18
1	B	2331	ARG	CA-C-N	6.70	126.73	119.89
1	B	2331	ARG	C-N-CA	6.70	126.73	119.89
1	C	1339	GLY	CA-C-N	-6.70	107.91	121.18
1	C	1339	GLY	C-N-CA	-6.70	107.91	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1339	GLY	CA-C-N	-6.68	107.95	121.18
1	B	1339	GLY	C-N-CA	-6.68	107.95	121.18
1	B	1078	ILE	CB-CA-C	-6.68	107.27	114.35
1	C	1078	ILE	CB-CA-C	-6.67	107.28	114.35
1	A	1078	ILE	CB-CA-C	-6.67	107.28	114.35
1	A	1390	GLU	N-CA-CB	-6.62	98.59	110.37
1	B	1390	GLU	N-CA-CB	-6.61	98.61	110.37
1	C	1390	GLU	N-CA-CB	-6.60	98.62	110.37
1	B	996	GLY	N-CA-C	-6.60	104.50	113.27
1	A	996	GLY	N-CA-C	-6.59	104.51	113.27
1	C	1000	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	1000	PHE	CA-CB-CG	6.56	120.36	113.80
1	C	996	GLY	N-CA-C	-6.55	104.56	113.27
1	B	1000	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	658	TYR	CA-C-O	-6.51	113.91	121.07
1	A	658	TYR	CA-C-O	-6.49	113.94	121.07
1	C	658	TYR	CA-C-O	-6.46	113.96	121.07
1	B	680	TYR	CA-CB-CG	6.37	125.36	113.90
1	A	680	TYR	CA-CB-CG	6.35	125.33	113.90
1	C	680	TYR	CA-CB-CG	6.35	125.33	113.90
1	A	997	PHE	CA-C-N	-6.31	111.85	120.44
1	A	997	PHE	C-N-CA	-6.31	111.85	120.44
1	B	997	PHE	CA-C-N	-6.31	111.86	120.44
1	B	997	PHE	C-N-CA	-6.31	111.86	120.44
1	C	997	PHE	CA-C-N	-6.30	111.87	120.44
1	C	997	PHE	C-N-CA	-6.30	111.87	120.44
1	B	644	VAL	CB-CA-C	-6.29	103.92	111.97
1	A	644	VAL	CB-CA-C	-6.26	103.96	111.97
1	A	1369	THR	N-CA-C	-6.24	104.36	112.23
1	C	1369	THR	N-CA-C	-6.24	104.37	112.23
1	B	1369	THR	N-CA-C	-6.23	104.38	112.23
1	C	644	VAL	CB-CA-C	-6.22	104.00	111.97
1	B	468	SER	CA-C-N	6.20	133.13	121.97
1	B	468	SER	C-N-CA	6.20	133.13	121.97
1	A	684	ALA	N-CA-C	-6.18	104.62	111.36
1	A	468	SER	CA-C-N	6.18	133.09	121.97
1	A	468	SER	C-N-CA	6.18	133.09	121.97
1	A	2332	PRO	N-CA-C	6.17	120.93	111.11
1	B	684	ALA	N-CA-C	-6.17	104.64	111.36
1	C	684	ALA	N-CA-C	-6.17	104.64	111.36
1	B	2332	PRO	N-CA-C	6.16	120.91	111.11
1	C	2332	PRO	N-CA-C	6.16	120.91	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1096	SER	N-CA-C	6.16	118.72	110.35
1	C	1382	ARG	CB-CA-C	6.16	119.72	109.56
1	C	468	SER	CA-C-N	6.15	133.04	121.97
1	C	468	SER	C-N-CA	6.15	133.04	121.97
1	A	1382	ARG	CB-CA-C	6.15	119.71	109.56
1	C	1096	SER	N-CA-C	6.15	118.71	110.35
1	B	1096	SER	N-CA-C	6.15	118.71	110.35
1	B	1382	ARG	CB-CA-C	6.13	119.68	109.56
1	A	651	THR	N-CA-C	6.10	120.34	113.02
1	B	651	THR	N-CA-C	6.09	120.32	113.02
1	C	651	THR	N-CA-C	6.07	120.30	113.02
1	B	973	PHE	CA-CB-CG	6.05	119.85	113.80
1	C	976	PHE	CB-CA-C	6.05	121.51	111.23
1	B	976	PHE	CB-CA-C	6.04	121.51	111.23
1	A	976	PHE	CB-CA-C	6.03	121.48	111.23
1	B	502	THR	N-CA-C	6.01	123.60	110.80
1	A	973	PHE	CA-CB-CG	6.00	119.81	113.80
1	A	502	THR	N-CA-C	5.98	123.54	110.80
1	C	502	THR	N-CA-C	5.98	123.54	110.80
1	B	1251	TRP	N-CA-C	-5.97	103.70	111.71
1	A	1251	TRP	N-CA-C	-5.97	103.71	111.71
1	B	2328	TYR	CA-C-O	-5.96	114.05	121.02
1	C	973	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	1391	PRO	N-CA-C	-5.96	102.88	111.22
1	A	2328	TYR	CA-C-O	-5.95	114.06	121.02
1	C	1251	TRP	N-CA-C	-5.95	103.74	111.71
1	C	2328	TYR	CA-C-O	-5.95	114.06	121.02
1	B	1337	ASN	CA-C-N	-5.94	110.20	121.54
1	B	1337	ASN	C-N-CA	-5.94	110.20	121.54
1	A	1094	ASN	N-CA-C	5.93	119.83	112.47
1	C	1391	PRO	N-CA-C	-5.93	102.91	111.22
1	A	1337	ASN	CA-C-N	-5.93	110.22	121.54
1	A	1337	ASN	C-N-CA	-5.93	110.22	121.54
1	B	1094	ASN	N-CA-C	5.92	119.82	112.47
1	C	1337	ASN	CA-C-N	-5.92	110.23	121.54
1	C	1337	ASN	C-N-CA	-5.92	110.23	121.54
1	A	1391	PRO	N-CA-C	-5.92	102.93	111.22
1	A	452	SER	N-CA-C	-5.92	103.80	111.02
1	C	452	SER	N-CA-C	-5.91	103.81	111.02
1	B	452	SER	N-CA-C	-5.91	103.81	111.02
1	C	1094	ASN	N-CA-C	5.91	119.79	112.47
1	B	485	PHE	N-CA-C	-5.90	104.43	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1001	GLY	CA-C-N	-5.90	112.86	120.65
1	C	1001	GLY	C-N-CA	-5.90	112.86	120.65
1	A	1001	GLY	CA-C-N	-5.89	112.88	120.65
1	A	1001	GLY	C-N-CA	-5.89	112.88	120.65
1	B	1001	GLY	CA-C-N	-5.88	112.89	120.65
1	B	1001	GLY	C-N-CA	-5.88	112.89	120.65
1	C	485	PHE	N-CA-C	-5.88	104.46	111.69
1	A	485	PHE	N-CA-C	-5.86	104.48	111.69
1	A	2200	GLU	N-CA-C	5.85	120.58	113.38
1	B	2200	GLU	N-CA-C	5.84	120.56	113.38
1	C	2200	GLU	N-CA-C	5.83	120.55	113.38
1	C	525	TYR	N-CA-CB	-5.82	101.26	110.22
1	A	525	TYR	N-CA-CB	-5.80	101.29	110.22
1	B	525	TYR	N-CA-CB	-5.79	101.31	110.22
1	B	658	TYR	N-CA-C	-5.76	103.99	111.02
1	A	658	TYR	N-CA-C	-5.74	104.02	111.02
1	C	658	TYR	N-CA-C	-5.73	104.02	111.02
1	A	639	ILE	N-CA-C	-5.58	105.08	110.72
1	C	639	ILE	N-CA-C	-5.58	105.09	110.72
1	B	639	ILE	N-CA-C	-5.54	105.12	110.72
1	B	487	LEU	N-CA-C	-5.54	105.14	111.07
1	A	487	LEU	N-CA-C	-5.53	105.15	111.07
1	C	487	LEU	N-CA-C	-5.53	105.15	111.07
1	C	976	PHE	N-CA-CB	-5.52	103.19	111.25
1	B	976	PHE	N-CA-CB	-5.52	103.19	111.25
1	A	976	PHE	N-CA-CB	-5.52	103.20	111.25
1	A	830	ILE	N-CA-C	-5.46	107.50	112.96
1	B	830	ILE	N-CA-C	-5.45	107.51	112.96
1	C	1828	ILE	N-CA-CB	-5.44	106.78	112.06
1	C	830	ILE	N-CA-C	-5.43	107.53	112.96
1	A	1828	ILE	N-CA-CB	-5.43	106.79	112.06
1	B	1828	ILE	N-CA-CB	-5.43	106.79	112.06
1	B	1698	ASP	CA-C-O	-5.42	114.68	120.42
1	C	679	LEU	N-CA-C	-5.41	105.55	111.82
1	A	679	LEU	N-CA-C	-5.41	105.55	111.82
1	B	679	LEU	N-CA-C	-5.40	105.55	111.82
1	A	1698	ASP	CA-C-O	-5.40	114.70	120.42
1	C	1698	ASP	CA-C-O	-5.39	114.71	120.42
1	A	992	LEU	N-CA-C	-5.37	104.84	111.33
1	B	2061	LEU	N-CA-C	-5.36	105.55	112.68
1	C	992	LEU	N-CA-C	-5.36	104.85	111.33
1	B	992	LEU	N-CA-C	-5.35	104.86	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2061	LEU	N-CA-C	-5.34	105.58	112.68
1	C	2061	LEU	N-CA-C	-5.34	105.58	112.68
1	A	484	ILE	N-CA-C	-5.33	98.25	109.34
1	C	484	ILE	N-CA-C	-5.33	98.25	109.34
1	B	484	ILE	N-CA-C	-5.32	98.28	109.34
1	C	486	GLY	N-CA-C	-5.27	106.02	112.77
1	B	486	GLY	N-CA-C	-5.25	106.05	112.77
1	A	486	GLY	N-CA-C	-5.25	106.06	112.77
1	B	1698	ASP	CB-CA-C	5.23	119.75	110.85
1	A	1698	ASP	CB-CA-C	5.22	119.72	110.85
1	C	1698	ASP	CB-CA-C	5.22	119.72	110.85
1	C	1268	LEU	N-CA-C	5.16	121.11	114.56
1	C	2375	ILE	N-CA-C	5.16	115.93	110.72
1	A	1268	LEU	N-CA-C	5.15	121.10	114.56
1	A	2349	ALA	CA-C-O	-5.14	113.15	120.51
1	B	2375	ILE	N-CA-C	5.14	115.92	110.72
1	C	2349	ALA	CA-C-O	-5.14	113.15	120.51
1	B	1268	LEU	N-CA-C	5.14	121.09	114.56
1	B	2349	ALA	CA-C-O	-5.13	113.17	120.51
1	A	2375	ILE	N-CA-C	5.13	115.90	110.72
1	B	501	ASP	N-CA-C	-5.13	100.95	109.46
1	C	501	ASP	N-CA-C	-5.12	100.96	109.46
1	A	501	ASP	N-CA-C	-5.11	100.97	109.46
1	C	1376	TYR	CB-CA-C	-5.05	102.26	110.85
1	A	1338	ARG	CA-C-N	-5.04	111.52	121.41
1	A	1338	ARG	C-N-CA	-5.04	111.52	121.41
1	B	1376	TYR	CB-CA-C	-5.04	102.27	110.85
1	A	1376	TYR	CB-CA-C	-5.04	102.28	110.85
1	B	1338	ARG	CA-C-N	-5.04	111.53	121.41
1	B	1338	ARG	C-N-CA	-5.04	111.53	121.41
1	C	1338	ARG	CA-C-N	-5.03	111.54	121.41
1	C	1338	ARG	C-N-CA	-5.03	111.54	121.41

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	GLU	Mainchain
1	A	1330	ARG	Sidechain
1	A	1373	ARG	Sidechain
1	A	1375	ARG	Sidechain
1	A	1382	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2033	ARG	Sidechain
1	A	2082	ARG	Sidechain
1	A	2157	ARG	Sidechain
1	A	2369	ARG	Sidechain
1	A	2373	ARG	Sidechain
1	A	285	CYS	Peptide
1	A	493	THR	Mainchain
1	A	503	ARG	Sidechain
1	A	681	ARG	Sidechain
1	B	1071	GLU	Mainchain
1	B	1330	ARG	Sidechain
1	B	1373	ARG	Sidechain
1	B	1375	ARG	Sidechain
1	B	1382	ARG	Sidechain
1	B	2033	ARG	Sidechain
1	B	2082	ARG	Sidechain
1	B	2157	ARG	Sidechain
1	B	2369	ARG	Sidechain
1	B	2373	ARG	Sidechain
1	B	285	CYS	Peptide
1	B	493	THR	Mainchain
1	B	503	ARG	Sidechain
1	B	681	ARG	Sidechain
1	C	1071	GLU	Mainchain
1	C	1330	ARG	Sidechain
1	C	1373	ARG	Sidechain
1	C	1375	ARG	Sidechain
1	C	1382	ARG	Sidechain
1	C	2033	ARG	Sidechain
1	C	2082	ARG	Sidechain
1	C	2157	ARG	Sidechain
1	C	2369	ARG	Sidechain
1	C	2373	ARG	Sidechain
1	C	285	CYS	Peptide
1	C	493	THR	Mainchain
1	C	503	ARG	Sidechain
1	C	681	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14835	0	14152	471	0
1	B	14835	0	14152	467	0
1	C	14835	0	14152	466	0
All	All	44505	0	42456	1369	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 16.

All (1369) 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:C:477:TRP:HH2	1:C:562:GLN:HE21	1.05	0.99
1:A:477:TRP:HH2	1:A:562:GLN:HE21	1.05	0.99
1:B:495:ILE:C	1:B:497:TRP:H	1.71	0.99
1:B:477:TRP:HH2	1:B:562:GLN:HE21	1.05	0.98
1:A:688:TRP:HA	1:A:760:LEU:HD21	1.45	0.97
1:A:495:ILE:C	1:A:497:TRP:H	1.71	0.96
1:A:1871:PRO:HG3	1:C:2064:TRP:CD1	2.01	0.96
1:C:688:TRP:HA	1:C:760:LEU:HD21	1.45	0.96
1:C:495:ILE:C	1:C:497:TRP:H	1.71	0.95
1:B:688:TRP:HA	1:B:760:LEU:HD21	1.45	0.95
1:A:2064:TRP:CD1	1:B:1871:PRO:HG3	2.01	0.95
1:B:2064:TRP:CD1	1:C:1871:PRO:HG3	2.01	0.94
1:A:2352:PHE:HD2	1:A:2355:GLY:H	1.08	0.94
1:B:1380:ILE:HD12	1:B:1405:MET:HA	1.50	0.94
1:C:1380:ILE:HD12	1:C:1405:MET:HA	1.50	0.93
1:B:2352:PHE:HD2	1:B:2355:GLY:H	1.08	0.93
1:A:1259:GLY:HA2	1:A:1262:LEU:HB2	1.52	0.92
1:C:2352:PHE:HD2	1:C:2355:GLY:H	1.08	0.92
1:C:1259:GLY:HA2	1:C:1262:LEU:HB2	1.52	0.91
1:B:1259:GLY:HA2	1:B:1262:LEU:HB2	1.52	0.91
1:B:1016:ARG:NH1	1:B:1106:TYR:HB3	1.87	0.90
1:A:1380:ILE:HD12	1:A:1405:MET:HA	1.50	0.90
1:C:1016:ARG:NH1	1:C:1106:TYR:HB3	1.86	0.90
1:B:1176:MET:HE3	1:B:1179:LEU:HD22	1.52	0.90
1:A:1176:MET:HE3	1:A:1179:LEU:HD22	1.52	0.89
1:A:2352:PHE:CD2	1:A:2355:GLY:N	2.41	0.89
1:B:2352:PHE:CE2	1:B:2354:GLY:HA3	2.08	0.89
1:C:640:PHE:O	1:C:644:VAL:HG23	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1176:MET:HE3	1:C:1179:LEU:HD22	1.52	0.88
1:C:2352:PHE:CD2	1:C:2355:GLY:N	2.41	0.88
1:A:1016:ARG:NH1	1:A:1106:TYR:HB3	1.87	0.88
1:A:460:THR:O	1:A:464:PHE:HD1	1.56	0.88
1:A:2352:PHE:CE2	1:A:2354:GLY:HA3	2.08	0.88
1:C:460:THR:O	1:C:464:PHE:HD1	1.56	0.88
1:B:640:PHE:O	1:B:644:VAL:HG23	1.74	0.87
1:C:2352:PHE:CE2	1:C:2354:GLY:HA3	2.08	0.87
1:A:685:TYR:HA	1:A:688:TRP:HE3	1.39	0.87
1:B:2352:PHE:CD2	1:B:2355:GLY:N	2.41	0.87
1:C:685:TYR:HA	1:C:688:TRP:HE3	1.39	0.87
1:B:460:THR:O	1:B:464:PHE:HD1	1.56	0.87
1:B:1827:TYR:HB2	1:B:1953:ASN:ND2	1.90	0.87
1:A:640:PHE:O	1:A:644:VAL:HG23	1.74	0.86
1:A:2194:ARG:HB3	1:A:2195:PRO:HD2	1.58	0.85
1:B:685:TYR:HA	1:B:688:TRP:HE3	1.39	0.85
1:B:2001:MET:HE2	1:B:2413:GLU:OE2	1.76	0.85
1:C:2194:ARG:HB3	1:C:2195:PRO:HD2	1.58	0.85
1:A:460:THR:HG22	1:A:464:PHE:HE1	1.41	0.85
1:A:687:PHE:HB2	1:A:760:LEU:CD1	2.06	0.85
1:A:1207:LEU:HD12	1:A:1219:HIS:CE1	2.11	0.85
1:A:2001:MET:HE2	1:A:2413:GLU:OE2	1.76	0.85
1:C:1827:TYR:HB2	1:C:1953:ASN:ND2	1.90	0.85
1:A:1827:TYR:HB2	1:A:1953:ASN:ND2	1.90	0.85
1:B:1207:LEU:HD12	1:B:1219:HIS:CE1	2.11	0.85
1:B:2063:LEU:O	1:B:2067:LEU:HG	1.77	0.84
1:C:2001:MET:HE2	1:C:2413:GLU:OE2	1.76	0.84
1:B:2194:ARG:HB3	1:B:2195:PRO:HD2	1.58	0.84
1:C:2063:LEU:O	1:C:2067:LEU:HG	1.77	0.84
1:C:1207:LEU:HD12	1:C:1219:HIS:CE1	2.11	0.84
1:B:687:PHE:HB2	1:B:760:LEU:CD1	2.06	0.84
1:C:460:THR:HG22	1:C:464:PHE:HE1	1.41	0.84
1:C:687:PHE:HB2	1:C:760:LEU:CD1	2.06	0.83
1:A:2063:LEU:O	1:A:2067:LEU:HG	1.77	0.83
1:A:225:THR:HA	1:A:577:ARG:HG3	1.61	0.83
1:A:991:PHE:HA	1:A:994:ASP:HB3	1.61	0.83
1:B:460:THR:HG22	1:B:464:PHE:HE1	1.41	0.82
1:B:991:PHE:HA	1:B:994:ASP:HB3	1.61	0.82
1:B:997:PHE:CZ	1:B:1123:VAL:HG13	2.15	0.82
1:B:225:THR:HA	1:B:577:ARG:HG3	1.61	0.81
1:B:483:SER:OG	1:B:486:GLY:N	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:CYS:O	1:C:497:TRP:HB2	1.80	0.81
1:C:997:PHE:CZ	1:C:1123:VAL:HG13	2.15	0.81
1:A:483:SER:OG	1:A:486:GLY:N	2.12	0.81
1:A:997:PHE:CZ	1:A:1123:VAL:HG13	2.15	0.81
1:C:225:THR:HA	1:C:577:ARG:HG3	1.61	0.81
1:C:477:TRP:CH2	1:C:562:GLN:NE2	2.47	0.81
1:C:483:SER:OG	1:C:486:GLY:N	2.12	0.81
1:B:687:PHE:HB2	1:B:760:LEU:HD11	1.63	0.81
1:B:2352:PHE:HD2	1:B:2355:GLY:N	1.77	0.81
1:C:2352:PHE:HD2	1:C:2355:GLY:N	1.77	0.81
1:A:494:CYS:O	1:A:497:TRP:HB2	1.80	0.81
1:B:1626:GLN:HG3	1:B:1638:PRO:HG3	1.62	0.81
1:C:1626:GLN:HG3	1:C:1638:PRO:HG3	1.62	0.81
1:B:494:CYS:O	1:B:497:TRP:HB2	1.80	0.81
1:B:1095:LEU:HD23	1:B:1096:SER:N	1.96	0.81
1:C:991:PHE:HA	1:C:994:ASP:HB3	1.61	0.81
1:C:1095:LEU:HD23	1:C:1096:SER:N	1.96	0.80
1:A:687:PHE:HB2	1:A:760:LEU:HD11	1.63	0.80
1:A:1095:LEU:HD23	1:A:1096:SER:N	1.96	0.80
1:A:1871:PRO:HG3	1:C:2064:TRP:NE1	1.97	0.80
1:C:687:PHE:HB2	1:C:760:LEU:HD11	1.63	0.79
1:A:644:VAL:O	1:A:648:VAL:HG23	1.82	0.79
1:A:690:THR:O	1:A:692:THR:N	2.16	0.79
1:A:1626:GLN:HG3	1:A:1638:PRO:HG3	1.62	0.79
1:C:690:THR:O	1:C:692:THR:N	2.16	0.79
1:B:644:VAL:O	1:B:648:VAL:HG23	1.82	0.79
1:A:2064:TRP:NE1	1:B:1871:PRO:HG3	1.97	0.79
1:C:644:VAL:O	1:C:648:VAL:HG23	1.82	0.79
1:B:690:THR:O	1:B:692:THR:N	2.16	0.78
1:B:2064:TRP:NE1	1:C:1871:PRO:HG3	1.97	0.78
1:B:483:SER:C	1:B:485:PHE:N	2.35	0.78
1:B:477:TRP:CH2	1:B:562:GLN:NE2	2.47	0.77
1:C:492:LEU:HD23	1:C:492:LEU:O	1.84	0.77
1:A:477:TRP:CH2	1:A:562:GLN:NE2	2.47	0.77
1:B:492:LEU:O	1:B:492:LEU:HD23	1.84	0.76
1:B:1016:ARG:HH12	1:B:1106:TYR:HB3	1.50	0.76
1:A:2352:PHE:HD2	1:A:2355:GLY:N	1.77	0.76
1:A:529:MET:HG2	1:A:548:TRP:HZ3	1.51	0.76
1:B:529:MET:HG2	1:B:548:TRP:HZ3	1.51	0.76
1:C:483:SER:HB2	1:C:485:PHE:HD1	1.51	0.76
1:A:460:THR:O	1:A:464:PHE:CD1	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD23	1:A:492:LEU:O	1.84	0.75
1:C:483:SER:C	1:C:485:PHE:N	2.35	0.75
1:A:1016:ARG:HH12	1:A:1106:TYR:HB3	1.49	0.75
1:A:483:SER:HB2	1:A:485:PHE:HD1	1.51	0.75
1:C:529:MET:HG2	1:C:548:TRP:HZ3	1.51	0.75
1:A:638:PHE:HB2	1:A:763:PHE:HZ	1.52	0.75
1:B:495:ILE:C	1:B:497:TRP:N	2.39	0.75
1:C:1330:ARG:O	1:C:1331:SER:C	2.30	0.75
1:B:1831:LEU:HD12	1:B:1831:LEU:O	1.87	0.74
1:A:649:VAL:HG11	1:A:752:LEU:HD22	1.69	0.74
1:C:649:VAL:HG11	1:C:752:LEU:HD22	1.69	0.74
1:C:1831:LEU:HD12	1:C:1831:LEU:O	1.87	0.74
1:B:638:PHE:HB2	1:B:763:PHE:HZ	1.52	0.73
1:C:1092:LEU:HD13	1:C:1243:ILE:HG13	1.70	0.73
1:A:1330:ARG:O	1:A:1331:SER:C	2.30	0.73
1:A:1831:LEU:HD12	1:A:1831:LEU:O	1.87	0.73
1:A:849:LEU:HD13	1:A:882:VAL:HB	1.71	0.73
1:B:649:VAL:HG11	1:B:752:LEU:HD22	1.70	0.73
1:B:1244:PHE:O	1:B:1247:VAL:HG22	1.88	0.73
1:C:638:PHE:HB2	1:C:763:PHE:HZ	1.52	0.73
1:C:1016:ARG:HH12	1:C:1106:TYR:HB3	1.50	0.73
1:C:460:THR:O	1:C:464:PHE:CD1	2.39	0.73
1:B:849:LEU:HD13	1:B:882:VAL:HB	1.71	0.73
1:C:483:SER:O	1:C:487:LEU:N	2.21	0.73
1:B:483:SER:O	1:B:487:LEU:N	2.22	0.73
1:B:1092:LEU:HD13	1:B:1243:ILE:HG13	1.70	0.73
1:C:849:LEU:HD13	1:C:882:VAL:HB	1.71	0.73
1:A:1092:LEU:HD13	1:A:1243:ILE:HG13	1.70	0.73
1:B:483:SER:HB2	1:B:485:PHE:HD1	1.51	0.73
1:B:1330:ARG:O	1:B:1331:SER:C	2.30	0.72
1:C:1244:PHE:O	1:C:1247:VAL:HG22	1.88	0.72
1:A:1244:PHE:O	1:A:1247:VAL:HG22	1.88	0.72
1:B:460:THR:O	1:B:464:PHE:CD1	2.39	0.72
1:A:495:ILE:C	1:A:497:TRP:N	2.39	0.72
1:B:851:ILE:HD11	1:B:1062:VAL:HG11	1.72	0.72
1:C:1207:LEU:CD1	1:C:1219:HIS:ND1	2.53	0.71
1:A:483:SER:C	1:A:485:PHE:N	2.35	0.71
1:A:1016:ARG:NE	1:A:1020:LEU:HD12	2.05	0.71
1:A:483:SER:O	1:A:487:LEU:N	2.21	0.71
1:A:851:ILE:HD11	1:A:1062:VAL:HG11	1.72	0.71
1:A:638:PHE:HB2	1:A:763:PHE:CZ	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:LEU:CD1	1:A:1219:HIS:ND1	2.53	0.71
1:A:2250:ASN:HB2	1:A:2344:PHE:HD1	1.56	0.71
1:C:638:PHE:HB2	1:C:763:PHE:CZ	2.25	0.71
1:C:676:SER:HB3	1:C:679:LEU:HD23	1.73	0.71
1:C:851:ILE:HD11	1:C:1062:VAL:HG11	1.72	0.71
1:B:638:PHE:HB2	1:B:763:PHE:CZ	2.25	0.71
1:B:1207:LEU:CD1	1:B:1219:HIS:ND1	2.53	0.71
1:B:483:SER:O	1:B:486:GLY:N	2.25	0.70
1:B:1016:ARG:NE	1:B:1020:LEU:HD12	2.05	0.70
1:B:2250:ASN:HB2	1:B:2344:PHE:HD1	1.56	0.70
1:C:2250:ASN:HB2	1:C:2344:PHE:HD1	1.56	0.70
1:A:483:SER:O	1:A:486:GLY:N	2.25	0.70
1:C:483:SER:O	1:C:486:GLY:N	2.25	0.70
1:C:495:ILE:C	1:C:497:TRP:N	2.39	0.70
1:C:685:TYR:O	1:C:688:TRP:HB2	1.92	0.70
1:B:495:ILE:O	1:B:497:TRP:N	2.25	0.70
1:A:676:SER:HB3	1:A:679:LEU:HD23	1.73	0.69
1:B:1157:SER:C	1:B:1161:TYR:H	2.00	0.69
1:C:1016:ARG:NE	1:C:1020:LEU:HD12	2.05	0.69
1:B:676:SER:HB3	1:B:679:LEU:HD23	1.73	0.69
1:B:685:TYR:O	1:B:688:TRP:HB2	1.92	0.69
1:C:495:ILE:O	1:C:497:TRP:N	2.25	0.69
1:A:999:LYS:HZ2	1:A:1316:ILE:HD12	1.58	0.69
1:A:1157:SER:C	1:A:1161:TYR:H	2.00	0.69
1:B:2061:LEU:HG	1:B:2360:TYR:OH	1.92	0.69
1:B:647:LEU:O	1:B:651:THR:HG22	1.93	0.69
1:C:203:VAL:HA	1:C:556:VAL:HG22	1.75	0.69
1:C:1977:LYS:O	1:C:1981:ASN:HB2	1.93	0.69
1:C:2061:LEU:HG	1:C:2360:TYR:OH	1.92	0.69
1:A:685:TYR:O	1:A:688:TRP:HB2	1.92	0.69
1:A:2061:LEU:HG	1:A:2360:TYR:OH	1.92	0.68
1:C:647:LEU:O	1:C:651:THR:HG22	1.93	0.68
1:C:999:LYS:HZ2	1:C:1316:ILE:HD12	1.58	0.68
1:A:647:LEU:O	1:A:651:THR:HG22	1.93	0.68
1:B:1977:LYS:O	1:B:1981:ASN:HB2	1.93	0.68
1:A:998:TYR:O	1:A:999:LYS:C	2.37	0.68
1:B:999:LYS:HZ2	1:B:1316:ILE:HD12	1.58	0.68
1:A:1050:MET:HE1	1:A:1113:VAL:HG22	1.76	0.68
1:B:1694:PRO:HA	1:B:1699:LYS:HE2	1.76	0.68
1:C:1694:PRO:HA	1:C:1699:LYS:HE2	1.76	0.68
1:A:495:ILE:O	1:A:497:TRP:N	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:ASN:HB2	1:B:1303:ASP:HB2	1.76	0.67
1:C:1157:SER:C	1:C:1161:TYR:H	2.00	0.67
1:A:1977:LYS:O	1:A:1981:ASN:HB2	1.93	0.67
1:B:203:VAL:HA	1:B:556:VAL:HG22	1.75	0.67
1:B:1000:PHE:O	1:B:1001:GLY:C	2.37	0.67
1:C:1307:LEU:O	1:C:1311:VAL:HG22	1.95	0.67
1:A:1307:LEU:O	1:A:1311:VAL:HG22	1.95	0.67
1:A:203:VAL:HA	1:A:556:VAL:HG22	1.75	0.67
1:B:460:THR:HG22	1:B:464:PHE:CE1	2.28	0.67
1:B:1160:ASP:O	1:B:1164:SER:N	2.22	0.67
1:C:477:TRP:HH2	1:C:562:GLN:NE2	1.86	0.67
1:C:1050:MET:HE1	1:C:1113:VAL:HG22	1.76	0.66
1:B:1050:MET:HE1	1:B:1113:VAL:HG22	1.76	0.66
1:B:998:TYR:O	1:B:999:LYS:C	2.37	0.66
1:C:1082:SER:HB2	1:C:1249:LEU:HD22	1.77	0.66
1:A:686:ALA:O	1:A:687:PHE:C	2.38	0.66
1:B:861:ILE:HD12	1:B:861:ILE:H	1.61	0.66
1:C:1207:LEU:CD1	1:C:1219:HIS:CE1	2.79	0.66
1:C:460:THR:HG22	1:C:464:PHE:CE1	2.28	0.66
1:A:1160:ASP:O	1:A:1164:SER:N	2.22	0.66
1:B:1082:SER:HB2	1:B:1249:LEU:HD22	1.77	0.66
1:C:1000:PHE:O	1:C:1001:GLY:C	2.37	0.66
1:A:687:PHE:CB	1:A:760:LEU:CD1	2.74	0.66
1:A:1160:ASP:O	1:A:1161:TYR:C	2.39	0.66
1:B:687:PHE:CB	1:B:760:LEU:CD1	2.74	0.66
1:B:978:HIS:CG	1:B:979:SER:H	2.14	0.66
1:A:1299:ASN:HB2	1:A:1303:ASP:HB2	1.76	0.66
1:B:1207:LEU:CD1	1:B:1219:HIS:CE1	2.79	0.66
1:A:1694:PRO:HA	1:A:1699:LYS:HE2	1.76	0.65
1:A:1827:TYR:CB	1:A:1953:ASN:ND2	2.59	0.65
1:B:686:ALA:O	1:B:689:LEU:N	2.26	0.65
1:B:1409:ASP:HB3	1:B:1412:ASN:HB2	1.79	0.65
1:C:1299:ASN:HB2	1:C:1303:ASP:HB2	1.77	0.65
1:B:1016:ARG:CZ	1:B:1020:LEU:HD12	2.26	0.65
1:B:2210:TRP:C	1:B:2211:LEU:HD12	2.21	0.65
1:C:1016:ARG:CZ	1:C:1020:LEU:HD12	2.26	0.65
1:C:2210:TRP:C	1:C:2211:LEU:HD12	2.21	0.65
1:C:1409:ASP:HB3	1:C:1412:ASN:HB2	1.79	0.65
1:A:1207:LEU:CD1	1:A:1219:HIS:CE1	2.79	0.65
1:B:1307:LEU:O	1:B:1311:VAL:HG22	1.95	0.65
1:C:978:HIS:CG	1:C:979:SER:H	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:VAL:O	1:A:1334:ILE:C	2.40	0.65
1:B:686:ALA:O	1:B:687:PHE:C	2.38	0.65
1:C:998:TYR:O	1:C:999:LYS:C	2.37	0.65
1:A:2250:ASN:HB2	1:A:2344:PHE:CD1	2.32	0.65
1:C:1827:TYR:CB	1:C:1953:ASN:ND2	2.59	0.65
1:C:2250:ASN:HB2	1:C:2344:PHE:CD1	2.32	0.65
1:B:477:TRP:HH2	1:B:562:GLN:NE2	1.86	0.65
1:B:685:TYR:HA	1:B:688:TRP:CE3	2.28	0.65
1:C:2272:ILE:HG22	1:C:2273:ASN:H	1.62	0.65
1:A:2210:TRP:C	1:A:2211:LEU:HD12	2.21	0.65
1:A:685:TYR:HA	1:A:688:TRP:CE3	2.28	0.65
1:A:861:ILE:H	1:A:861:ILE:HD12	1.61	0.65
1:A:1249:LEU:HD21	1:A:1281:LEU:HD22	1.79	0.65
1:B:1827:TYR:CB	1:B:1953:ASN:ND2	2.59	0.65
1:B:2250:ASN:HB2	1:B:2344:PHE:CD1	2.32	0.65
1:A:978:HIS:CG	1:A:979:SER:H	2.14	0.64
1:A:982:ASP:O	1:A:983:ARG:C	2.41	0.64
1:C:686:ALA:O	1:C:687:PHE:C	2.38	0.64
1:A:460:THR:HG22	1:A:464:PHE:CE1	2.28	0.64
1:A:483:SER:C	1:A:485:PHE:H	2.05	0.64
1:B:982:ASP:O	1:B:983:ARG:C	2.41	0.64
1:C:687:PHE:CB	1:C:760:LEU:CD1	2.74	0.64
1:A:1082:SER:HB2	1:A:1249:LEU:HD22	1.77	0.64
1:A:1409:ASP:HB3	1:A:1412:ASN:HB2	1.79	0.64
1:C:1160:ASP:O	1:C:1161:TYR:C	2.39	0.64
1:C:483:SER:C	1:C:485:PHE:H	2.05	0.64
1:C:685:TYR:HA	1:C:688:TRP:CE3	2.28	0.64
1:A:1016:ARG:CZ	1:A:1020:LEU:HD12	2.26	0.64
1:A:2352:PHE:CE2	1:A:2354:GLY:CA	2.81	0.64
1:B:1333:VAL:O	1:B:1334:ILE:C	2.40	0.64
1:B:483:SER:C	1:B:485:PHE:H	2.05	0.64
1:B:1641:SER:HA	1:B:1656:PHE:HZ	1.63	0.64
1:C:861:ILE:HD12	1:C:861:ILE:H	1.61	0.64
1:A:997:PHE:CE2	1:A:1123:VAL:HG13	2.33	0.64
1:A:2272:ILE:HG22	1:A:2273:ASN:H	1.62	0.64
1:C:997:PHE:CE2	1:C:1123:VAL:HG13	2.33	0.64
1:A:1000:PHE:O	1:A:1001:GLY:C	2.37	0.64
1:C:1333:VAL:O	1:C:1334:ILE:C	2.40	0.64
1:C:2272:ILE:HG22	1:C:2273:ASN:N	2.13	0.64
1:A:1037:VAL:HG12	1:A:1040:ARG:HE	1.63	0.64
1:A:2272:ILE:HG22	1:A:2273:ASN:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2272:ILE:HG22	1:B:2273:ASN:H	1.62	0.64
1:B:2272:ILE:HG22	1:B:2273:ASN:N	2.13	0.64
1:C:1249:LEU:HD21	1:C:1281:LEU:HD22	1.79	0.64
1:B:2352:PHE:CE2	1:B:2354:GLY:CA	2.81	0.63
1:C:982:ASP:O	1:C:983:ARG:C	2.41	0.63
1:B:687:PHE:HD2	1:B:764:HIS:HE2	1.47	0.63
1:B:997:PHE:CE2	1:B:1123:VAL:HG13	2.33	0.63
1:B:1037:VAL:HG12	1:B:1040:ARG:HE	1.63	0.63
1:B:1095:LEU:HD23	1:B:1096:SER:H	1.62	0.63
1:C:1037:VAL:HG12	1:C:1040:ARG:HE	1.63	0.63
1:A:996:GLY:O	1:A:997:PHE:C	2.42	0.63
1:A:1909:ALA:O	1:A:1913:ILE:HG22	1.99	0.63
1:A:477:TRP:HH2	1:A:562:GLN:NE2	1.86	0.63
1:A:490:LEU:C	1:A:490:LEU:HD23	2.24	0.63
1:A:1095:LEU:HD23	1:A:1096:SER:H	1.62	0.63
1:B:1160:ASP:O	1:B:1161:TYR:C	2.39	0.63
1:B:1909:ALA:O	1:B:1913:ILE:HG22	1.99	0.63
1:C:687:PHE:HD2	1:C:764:HIS:HE2	1.47	0.63
1:A:1641:SER:HA	1:A:1656:PHE:HZ	1.63	0.63
1:B:1249:LEU:HD21	1:B:1281:LEU:HD22	1.79	0.63
1:C:1641:SER:HA	1:C:1656:PHE:HZ	1.63	0.63
1:C:996:GLY:O	1:C:997:PHE:C	2.42	0.62
1:C:1005:THR:O	1:C:1009:ILE:HD12	1.99	0.62
1:C:1909:ALA:O	1:C:1913:ILE:HG22	1.99	0.62
1:A:687:PHE:HD2	1:A:764:HIS:HE2	1.47	0.62
1:A:1871:PRO:HG3	1:C:2064:TRP:HE1	1.62	0.62
1:B:996:GLY:O	1:B:997:PHE:C	2.42	0.62
1:B:1888:ASP:HA	1:B:1891:LEU:HD13	1.81	0.62
1:C:483:SER:C	1:C:486:GLY:H	2.07	0.62
1:A:2064:TRP:HE1	1:B:1871:PRO:HG3	1.62	0.62
1:B:483:SER:C	1:B:486:GLY:H	2.07	0.62
1:C:490:LEU:HD23	1:C:490:LEU:C	2.24	0.62
1:C:1686:TRP:CH2	1:C:1698:ASP:HB3	2.35	0.62
1:A:483:SER:C	1:A:486:GLY:H	2.07	0.62
1:A:1207:LEU:HD11	1:A:1219:HIS:CG	2.35	0.62
1:B:1208:TYR:HE1	1:B:1219:HIS:NE2	1.98	0.62
1:C:1095:LEU:HD23	1:C:1096:SER:H	1.62	0.62
1:C:1208:TYR:HE1	1:C:1219:HIS:NE2	1.98	0.62
1:B:1005:THR:O	1:B:1009:ILE:HD12	2.00	0.62
1:B:1207:LEU:HD11	1:B:1219:HIS:CG	2.35	0.62
1:A:1208:TYR:HE1	1:A:1219:HIS:NE2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1207:LEU:HD11	1:C:1219:HIS:CG	2.35	0.62
1:A:1005:THR:O	1:A:1009:ILE:HD12	2.00	0.62
1:B:887:MET:HE3	1:B:887:MET:HA	1.82	0.62
1:A:686:ALA:O	1:A:689:LEU:N	2.26	0.62
1:A:1686:TRP:CZ2	1:A:1698:ASP:HB3	2.35	0.62
1:B:490:LEU:C	1:B:490:LEU:HD23	2.24	0.62
1:C:1005:THR:OG1	1:C:1116:LEU:HB3	2.00	0.62
1:B:1686:TRP:CH2	1:B:1698:ASP:HB3	2.35	0.61
1:C:1888:ASP:HA	1:C:1891:LEU:HD13	1.81	0.61
1:C:2352:PHE:CE2	1:C:2354:GLY:CA	2.81	0.61
1:B:2064:TRP:HE1	1:C:1871:PRO:HG3	1.63	0.61
1:A:2351:VAL:O	1:A:2352:PHE:C	2.43	0.61
1:B:1157:SER:O	1:B:1158:TYR:C	2.44	0.61
1:B:2351:VAL:O	1:B:2352:PHE:C	2.43	0.61
1:C:1157:SER:O	1:C:1158:TYR:C	2.44	0.61
1:C:1686:TRP:CZ2	1:C:1698:ASP:HB3	2.35	0.61
1:A:978:HIS:CG	1:A:979:SER:N	2.68	0.61
1:C:990:GLN:O	1:C:993:ILE:N	2.33	0.61
1:B:1005:THR:OG1	1:B:1116:LEU:HB3	2.00	0.61
1:B:1686:TRP:CZ2	1:B:1698:ASP:HB3	2.35	0.61
1:B:699:ILE:HD11	1:B:749:PRO:HB2	1.83	0.61
1:C:1635:LEU:HG	1:C:1639:LEU:HD12	1.83	0.61
1:A:699:ILE:HD11	1:A:749:PRO:HB2	1.83	0.61
1:A:1635:LEU:HG	1:A:1639:LEU:HD12	1.83	0.61
1:A:1157:SER:O	1:A:1158:TYR:C	2.44	0.61
1:A:2260:ILE:O	1:A:2264:ILE:HG22	2.01	0.61
1:C:699:ILE:HD11	1:C:749:PRO:HB2	1.83	0.61
1:C:887:MET:HE3	1:C:887:MET:HA	1.82	0.61
1:C:978:HIS:CG	1:C:979:SER:N	2.68	0.61
1:A:1686:TRP:CH2	1:A:1698:ASP:HB3	2.35	0.60
1:A:1888:ASP:HA	1:A:1891:LEU:HD13	1.81	0.60
1:C:494:CYS:HA	1:C:497:TRP:HD1	1.66	0.60
1:B:990:GLN:O	1:B:993:ILE:N	2.33	0.60
1:A:494:CYS:HA	1:A:497:TRP:HD1	1.66	0.60
1:A:1005:THR:OG1	1:A:1116:LEU:HB3	2.00	0.60
1:B:1635:LEU:HG	1:B:1639:LEU:HD12	1.83	0.60
1:C:1828:ILE:HG22	1:C:1828:ILE:O	2.01	0.60
1:C:2351:VAL:O	1:C:2352:PHE:C	2.43	0.60
1:A:887:MET:HE3	1:A:887:MET:HA	1.82	0.60
1:A:1828:ILE:HG22	1:A:1828:ILE:O	2.01	0.60
1:B:494:CYS:HA	1:B:497:TRP:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1871:PRO:O	1:C:1872:VAL:HG22	2.02	0.60
1:B:978:HIS:CG	1:B:979:SER:N	2.68	0.60
1:A:1157:SER:O	1:A:1160:ASP:N	2.34	0.60
1:B:1871:PRO:O	1:B:1872:VAL:HG22	2.02	0.60
1:C:1160:ASP:O	1:C:1164:SER:N	2.22	0.60
1:A:1871:PRO:O	1:A:1872:VAL:HG22	2.02	0.60
1:B:688:TRP:CZ2	1:B:764:HIS:HB3	2.37	0.60
1:B:1828:ILE:O	1:B:1828:ILE:HG22	2.01	0.60
1:B:2147:THR:HG23	1:B:2149:GLU:H	1.66	0.60
1:B:2260:ILE:O	1:B:2264:ILE:HG22	2.01	0.60
1:A:687:PHE:HD2	1:A:764:HIS:NE2	2.00	0.60
1:B:1242:GLN:HB2	1:B:1273:CYS:HA	1.84	0.60
1:B:2210:TRP:O	1:B:2211:LEU:HD12	2.02	0.60
1:C:1157:SER:O	1:C:1160:ASP:N	2.34	0.60
1:C:2147:THR:HG23	1:C:2149:GLU:H	1.66	0.60
1:C:1242:GLN:HB2	1:C:1273:CYS:HA	1.84	0.59
1:A:2210:TRP:O	1:A:2211:LEU:HD12	2.02	0.59
1:C:988:ALA:O	1:C:989:ILE:C	2.45	0.59
1:C:2260:ILE:O	1:C:2264:ILE:HG22	2.01	0.59
1:A:2147:THR:HG23	1:A:2149:GLU:H	1.66	0.59
1:A:688:TRP:CZ2	1:A:764:HIS:HB3	2.37	0.59
1:B:988:ALA:O	1:B:989:ILE:C	2.45	0.59
1:B:1157:SER:O	1:B:1160:ASP:N	2.34	0.59
1:A:1392:VAL:HG23	1:C:2033:ARG:H	1.67	0.59
1:B:1582:VAL:HA	1:B:1585:MET:HG2	1.85	0.59
1:B:2033:ARG:H	1:C:1392:VAL:HG23	1.67	0.59
1:C:1119:CYS:O	1:C:1123:VAL:HG23	2.03	0.59
1:A:1119:CYS:O	1:A:1123:VAL:HG23	2.03	0.59
1:B:1314:ILE:HA	1:B:1317:PHE:HE1	1.68	0.59
1:A:1314:ILE:HA	1:A:1317:PHE:HE1	1.68	0.59
1:A:1582:VAL:HA	1:A:1585:MET:HG2	1.85	0.59
1:C:649:VAL:HG11	1:C:752:LEU:CD2	2.33	0.59
1:C:2210:TRP:O	1:C:2211:LEU:HD12	2.02	0.59
1:B:2350:LYS:HG2	1:B:2353:LYS:HG3	1.84	0.59
1:A:1242:GLN:HB2	1:A:1273:CYS:HA	1.84	0.58
1:A:2033:ARG:H	1:B:1392:VAL:HG23	1.67	0.58
1:B:687:PHE:HD2	1:B:764:HIS:NE2	2.00	0.58
1:B:1119:CYS:O	1:B:1123:VAL:HG23	2.03	0.58
1:C:688:TRP:CZ2	1:C:764:HIS:HB3	2.37	0.58
1:C:1314:ILE:HA	1:C:1317:PHE:HE1	1.67	0.58
1:C:1887:ILE:O	1:C:1891:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:ALA:HA	1:A:1193:TYR:HD1	1.68	0.58
1:B:649:VAL:HG11	1:B:752:LEU:CD2	2.33	0.58
1:C:529:MET:HG2	1:C:548:TRP:CZ3	2.37	0.58
1:C:687:PHE:HD2	1:C:764:HIS:NE2	2.00	0.58
1:C:1190:ALA:HA	1:C:1193:TYR:HD1	1.68	0.58
1:A:649:VAL:HG11	1:A:752:LEU:CD2	2.33	0.58
1:A:2373:ARG:NH2	1:B:1986:PHE:CD2	2.71	0.58
1:C:1582:VAL:HA	1:C:1585:MET:HG2	1.85	0.58
1:C:2350:LYS:HG2	1:C:2353:LYS:HG3	1.84	0.58
1:B:1847:THR:O	1:B:1848:PHE:C	2.47	0.58
1:A:988:ALA:O	1:A:989:ILE:C	2.45	0.58
1:A:1887:ILE:O	1:A:1891:LEU:HD12	2.03	0.58
1:C:1838:ILE:HG21	1:C:1943:TYR:HB2	1.86	0.58
1:A:566:THR:O	1:A:569:VAL:HG12	2.03	0.58
1:B:1838:ILE:HG21	1:B:1943:TYR:HB2	1.86	0.58
1:A:1077:TRP:C	1:A:1079:PRO:HD2	2.29	0.58
1:A:1838:ILE:HG21	1:A:1943:TYR:HB2	1.86	0.58
1:A:2350:LYS:HG2	1:A:2353:LYS:HG3	1.84	0.58
1:B:566:THR:O	1:B:569:VAL:HG12	2.03	0.58
1:C:1266:ARG:HD2	1:C:1266:ARG:O	2.04	0.58
1:A:1266:ARG:HD2	1:A:1266:ARG:O	2.04	0.57
1:A:2194:ARG:HB3	1:A:2195:PRO:CD	2.33	0.57
1:B:1190:ALA:HA	1:B:1193:TYR:HD1	1.68	0.57
1:B:2387:GLU:HB2	1:C:1399:ARG:HD3	1.86	0.57
1:C:566:THR:O	1:C:569:VAL:HG12	2.03	0.57
1:C:688:TRP:N	1:C:760:LEU:HD11	2.19	0.57
1:C:1077:TRP:C	1:C:1079:PRO:HD2	2.29	0.57
1:B:1077:TRP:C	1:B:1079:PRO:HD2	2.29	0.57
1:B:1887:ILE:O	1:B:1891:LEU:HD12	2.03	0.57
1:C:988:ALA:O	1:C:990:GLN:N	2.38	0.57
1:C:2084:SER:HB3	1:C:2090:PRO:HA	1.87	0.57
1:B:688:TRP:N	1:B:760:LEU:HD11	2.20	0.57
1:C:1626:GLN:HG2	1:C:1634:THR:HG23	1.87	0.57
1:A:1399:ARG:HD3	1:C:2387:GLU:HB2	1.86	0.57
1:A:1986:PHE:CD2	1:C:2373:ARG:NH2	2.71	0.57
1:B:529:MET:HG2	1:B:548:TRP:CZ3	2.37	0.57
1:B:2373:ARG:NH2	1:C:1986:PHE:CD2	2.71	0.57
1:B:2325:ASN:O	1:B:2326:THR:HG22	2.05	0.57
1:C:1847:THR:O	1:C:1848:PHE:C	2.47	0.57
1:A:2325:ASN:O	1:A:2326:THR:HG22	2.05	0.57
1:C:686:ALA:O	1:C:689:LEU:N	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TRP:N	1:A:760:LEU:HD11	2.20	0.57
1:B:1626:GLN:HG2	1:B:1634:THR:HG23	1.87	0.57
1:A:2387:GLU:HB2	1:B:1399:ARG:HD3	1.86	0.56
1:C:1179:LEU:O	1:C:1183:ILE:HG13	2.05	0.56
1:A:1827:TYR:HB2	1:A:1953:ASN:HD22	1.70	0.56
1:B:939:ILE:O	1:B:943:ILE:HG23	2.05	0.56
1:B:2084:SER:HB3	1:B:2090:PRO:HA	1.87	0.56
1:A:1007:ILE:HG12	1:A:1308:SER:HB2	1.87	0.56
1:A:1831:LEU:O	1:A:1831:LEU:CD1	2.54	0.56
1:B:1007:ILE:HG12	1:B:1308:SER:HB2	1.87	0.56
1:A:558:ILE:HD12	1:A:559:LEU:N	2.21	0.56
1:A:988:ALA:O	1:A:990:GLN:N	2.38	0.56
1:B:558:ILE:HD12	1:B:559:LEU:N	2.21	0.56
1:B:988:ALA:O	1:B:990:GLN:N	2.38	0.56
1:C:2325:ASN:O	1:C:2326:THR:HG22	2.05	0.56
1:B:1266:ARG:HD2	1:B:1266:ARG:O	2.04	0.56
1:C:1007:ILE:HG12	1:C:1308:SER:HB2	1.88	0.56
1:A:939:ILE:O	1:A:943:ILE:HG23	2.05	0.56
1:B:1193:TYR:O	1:B:1197:THR:HG22	2.06	0.56
1:A:1179:LEU:O	1:A:1183:ILE:HG13	2.05	0.56
1:A:1271:ILE:CG1	1:A:1293:VAL:HG13	2.36	0.56
1:C:1271:ILE:CG1	1:C:1293:VAL:HG13	2.36	0.56
1:B:1271:ILE:CG1	1:B:1293:VAL:HG13	2.36	0.56
1:A:1193:TYR:O	1:A:1197:THR:HG22	2.06	0.56
1:A:990:GLN:O	1:A:993:ILE:N	2.33	0.56
1:A:1626:GLN:HG2	1:A:1634:THR:HG23	1.87	0.56
1:C:991:PHE:HD1	1:C:994:ASP:HB3	1.71	0.56
1:C:1193:TYR:O	1:C:1197:THR:HG22	2.06	0.56
1:C:1831:LEU:O	1:C:1831:LEU:CD1	2.54	0.56
1:A:2155:ARG:HD3	1:A:2333:TYR:HD2	1.71	0.55
1:B:1884:ALA:HA	1:B:1887:ILE:HD12	1.88	0.55
1:C:2194:ARG:HB3	1:C:2195:PRO:CD	2.33	0.55
1:A:2084:SER:HB3	1:A:2090:PRO:HA	1.87	0.55
1:B:1827:TYR:HB2	1:B:1953:ASN:HD22	1.70	0.55
1:C:939:ILE:O	1:C:943:ILE:HG23	2.05	0.55
1:C:1827:TYR:HB2	1:C:1953:ASN:HD22	1.70	0.55
1:A:1827:TYR:CB	1:A:1953:ASN:HD22	2.20	0.55
1:B:1693:ASP:OD1	1:B:1699:LYS:HD3	2.07	0.55
1:C:558:ILE:HD12	1:C:559:LEU:N	2.21	0.55
1:C:1884:ALA:HA	1:C:1887:ILE:HD12	1.88	0.55
1:A:1870:ILE:HG22	1:A:1872:VAL:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1179:LEU:O	1:B:1183:ILE:HG13	2.06	0.55
1:B:1831:LEU:O	1:B:1831:LEU:CD1	2.54	0.55
1:B:1870:ILE:HG22	1:B:1872:VAL:H	1.71	0.55
1:C:1266:ARG:NE	1:C:1291:CYS:SG	2.80	0.55
1:A:554:HIS:O	1:A:558:ILE:HG13	2.07	0.55
1:A:996:GLY:O	1:A:999:LYS:N	2.40	0.55
1:B:1870:ILE:CG2	1:B:1871:PRO:HD2	2.37	0.55
1:A:1239:VAL:O	1:A:1242:GLN:HG3	2.06	0.55
1:A:1266:ARG:NE	1:A:1291:CYS:SG	2.80	0.55
1:B:991:PHE:HD1	1:B:994:ASP:HB3	1.71	0.55
1:C:554:HIS:O	1:C:558:ILE:HG13	2.07	0.55
1:C:996:GLY:O	1:C:999:LYS:N	2.40	0.55
1:C:2155:ARG:HD3	1:C:2333:TYR:HD2	1.71	0.55
1:A:529:MET:HG2	1:A:548:TRP:CZ3	2.37	0.55
1:A:1693:ASP:OD1	1:A:1699:LYS:HD3	2.07	0.55
1:B:544:VAL:HG13	1:B:546:ILE:H	1.72	0.55
1:B:1666:CYS:O	1:B:1670:ILE:HG22	2.07	0.55
1:C:1693:ASP:OD1	1:C:1699:LYS:HD3	2.07	0.55
1:C:1870:ILE:HG22	1:C:1872:VAL:H	1.72	0.55
1:A:1870:ILE:CG2	1:A:1871:PRO:HD2	2.37	0.55
1:A:544:VAL:HG13	1:A:546:ILE:H	1.72	0.54
1:A:1884:ALA:HA	1:A:1887:ILE:HD12	1.88	0.54
1:B:224:SER:CB	1:B:573:LEU:HB3	2.37	0.54
1:B:1827:TYR:CB	1:B:1953:ASN:HD22	2.20	0.54
1:B:2155:ARG:HD3	1:B:2333:TYR:HD2	1.71	0.54
1:C:2019:ILE:O	1:C:2023:ARG:HG2	2.07	0.54
1:B:1239:VAL:O	1:B:1242:GLN:HG3	2.06	0.54
1:B:1266:ARG:NE	1:B:1291:CYS:SG	2.80	0.54
1:C:224:SER:CB	1:C:573:LEU:HB3	2.37	0.54
1:A:1847:THR:O	1:A:1848:PHE:C	2.47	0.54
1:A:2019:ILE:O	1:A:2023:ARG:HG2	2.07	0.54
1:B:977:HIS:HB2	1:B:980:HIS:ND1	2.22	0.54
1:C:1239:VAL:O	1:C:1242:GLN:HG3	2.06	0.54
1:A:1654:LYS:HA	1:A:1657:TRP:HD1	1.73	0.54
1:A:991:PHE:HA	1:A:995:TYR:H	1.73	0.54
1:B:554:HIS:O	1:B:558:ILE:HG13	2.07	0.54
1:B:996:GLY:O	1:B:999:LYS:N	2.40	0.54
1:C:977:HIS:HB2	1:C:980:HIS:ND1	2.22	0.54
1:A:1311:VAL:HA	1:A:1314:ILE:HG22	1.90	0.54
1:B:2019:ILE:O	1:B:2023:ARG:HG2	2.07	0.54
1:C:991:PHE:HA	1:C:995:TYR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1870:ILE:CG2	1:C:1871:PRO:HD2	2.37	0.54
1:A:1666:CYS:O	1:A:1670:ILE:HG22	2.07	0.54
1:B:1654:LYS:HA	1:B:1657:TRP:HD1	1.73	0.54
1:C:1666:CYS:O	1:C:1670:ILE:HG22	2.07	0.54
1:A:224:SER:CB	1:A:573:LEU:HB3	2.37	0.54
1:A:947:PHE:O	1:A:951:VAL:HG22	2.08	0.54
1:A:977:HIS:HB2	1:A:980:HIS:ND1	2.22	0.54
1:A:991:PHE:HD1	1:A:994:ASP:HB3	1.71	0.54
1:B:1211:ASN:HB3	1:B:1330:ARG:HD3	1.90	0.54
1:B:1717:LEU:HD12	1:B:1717:LEU:C	2.33	0.54
1:A:1883:LEU:HA	1:A:1886:ILE:HD12	1.90	0.54
1:B:947:PHE:O	1:B:951:VAL:HG22	2.08	0.54
1:B:991:PHE:HA	1:B:995:TYR:H	1.73	0.54
1:B:1121:LEU:HD13	1:B:1121:LEU:O	2.08	0.54
1:B:2194:ARG:HB3	1:B:2195:PRO:CD	2.33	0.54
1:C:307:TRP:O	1:C:311:ALA:CB	2.56	0.53
1:A:224:SER:O	1:A:577:ARG:HB2	2.09	0.53
1:A:488:ILE:O	1:A:489:LEU:C	2.52	0.53
1:A:1207:LEU:HD11	1:A:1219:HIS:ND1	2.24	0.53
1:C:1827:TYR:CB	1:C:1953:ASN:HD22	2.20	0.53
1:A:526:PHE:C	1:A:528:SER:H	2.16	0.53
1:A:1335:LEU:HD23	1:A:1336:ALA:N	2.23	0.53
1:A:1717:LEU:C	1:A:1717:LEU:HD12	2.33	0.53
1:A:1871:PRO:HG3	1:C:2064:TRP:HD1	1.69	0.53
1:B:224:SER:O	1:B:577:ARG:HB2	2.09	0.53
1:C:1211:ASN:HB3	1:C:1330:ARG:HD3	1.90	0.53
1:C:1654:LYS:HA	1:C:1657:TRP:HD1	1.73	0.53
1:C:1717:LEU:C	1:C:1717:LEU:HD12	2.33	0.53
1:C:1883:LEU:HA	1:C:1886:ILE:HD12	1.90	0.53
1:A:1211:ASN:HB3	1:A:1330:ARG:HD3	1.90	0.53
1:A:307:TRP:O	1:A:311:ALA:CB	2.56	0.53
1:A:1121:LEU:O	1:A:1121:LEU:HD13	2.08	0.53
1:B:1335:LEU:HD23	1:B:1336:ALA:N	2.23	0.53
1:C:544:VAL:HG13	1:C:546:ILE:H	1.72	0.53
1:C:1335:LEU:HD23	1:C:1336:ALA:N	2.23	0.53
1:A:1267:GLN:O	1:A:1268:LEU:HD22	2.08	0.53
1:C:1121:LEU:HD13	1:C:1121:LEU:O	2.08	0.53
1:C:1311:VAL:HA	1:C:1314:ILE:HG22	1.90	0.53
1:B:823:TRP:HE1	1:B:954:ARG:HD2	1.74	0.53
1:C:1267:GLN:O	1:C:1268:LEU:HD22	2.08	0.53
1:B:1207:LEU:CD1	1:B:1219:HIS:CG	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ARG:HD2	1:A:1218:GLU:HB2	1.91	0.52
1:B:526:PHE:C	1:B:528:SER:H	2.16	0.52
1:B:1311:VAL:HA	1:B:1314:ILE:HG22	1.89	0.52
1:C:224:SER:O	1:C:577:ARG:HB2	2.09	0.52
1:A:484:ILE:O	1:A:488:ILE:HG13	2.10	0.52
1:B:307:TRP:O	1:B:311:ALA:CB	2.56	0.52
1:C:526:PHE:C	1:C:528:SER:H	2.16	0.52
1:C:1250:SER:HB3	1:C:1284:LEU:HD11	1.91	0.52
1:B:516:TYR:CE1	1:B:519:PHE:HE2	2.27	0.52
1:C:947:PHE:O	1:C:951:VAL:HG22	2.08	0.52
1:A:225:THR:HA	1:A:577:ARG:CG	2.38	0.52
1:A:1160:ASP:HA	1:A:1163:LYS:HB2	1.92	0.52
1:B:1267:GLN:O	1:B:1268:LEU:HD22	2.08	0.52
1:C:1215:ARG:HD2	1:C:1218:GLU:HB2	1.91	0.52
1:A:1271:ILE:HG23	1:A:1272:THR:H	1.74	0.52
1:B:680:TYR:OH	1:B:953:TYR:HB3	2.09	0.52
1:C:1207:LEU:HD11	1:C:1219:HIS:ND1	2.24	0.52
1:A:823:TRP:HE1	1:A:954:ARG:HD2	1.74	0.52
1:A:1585:MET:HB2	1:A:1589:VAL:HG13	1.91	0.52
1:A:516:TYR:CE1	1:A:519:PHE:HE2	2.27	0.52
1:C:484:ILE:O	1:C:488:ILE:HG13	2.10	0.52
1:C:1585:MET:HB2	1:C:1589:VAL:HG13	1.91	0.52
1:B:1302:PHE:HA	1:B:1305:ILE:HD11	1.92	0.52
1:C:680:TYR:OH	1:C:953:TYR:HB3	2.09	0.52
1:A:1826:ARG:HB2	1:A:1826:ARG:NH1	2.25	0.52
1:B:224:SER:O	1:B:574:ARG:HA	2.10	0.52
1:B:1271:ILE:HG23	1:B:1272:THR:H	1.74	0.52
1:B:1272:THR:O	1:B:1273:CYS:C	2.53	0.52
1:C:1207:LEU:CD1	1:C:1219:HIS:CG	2.92	0.52
1:B:1883:LEU:HA	1:B:1886:ILE:HD12	1.90	0.51
1:C:516:TYR:CE1	1:C:519:PHE:HE2	2.27	0.51
1:C:1160:ASP:HA	1:C:1163:LYS:HB2	1.92	0.51
1:C:1272:THR:O	1:C:1273:CYS:C	2.53	0.51
1:A:680:TYR:OH	1:A:953:TYR:HB3	2.09	0.51
1:A:1207:LEU:CD1	1:A:1219:HIS:CG	2.92	0.51
1:A:2109:ILE:HG21	1:A:2151:ILE:HB	1.92	0.51
1:B:484:ILE:O	1:B:488:ILE:HG13	2.10	0.51
1:B:1585:MET:HB2	1:B:1589:VAL:HG13	1.91	0.51
1:C:224:SER:O	1:C:574:ARG:HA	2.10	0.51
1:C:1302:PHE:HA	1:C:1305:ILE:HD11	1.92	0.51
1:A:1302:PHE:HA	1:A:1305:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1842:CYS:HA	1:A:1845:ILE:HG22	1.91	0.51
1:C:1271:ILE:HG23	1:C:1272:THR:H	1.74	0.51
1:A:224:SER:O	1:A:574:ARG:HA	2.10	0.51
1:B:630:LEU:O	1:B:634:VAL:HG23	2.11	0.51
1:B:657:PHE:HD2	1:B:728:ILE:HD13	1.76	0.51
1:C:713:TRP:NE1	1:C:717:ASN:HD21	2.09	0.51
1:C:1380:ILE:CD1	1:C:1405:MET:HA	2.33	0.51
1:B:1160:ASP:HA	1:B:1163:LYS:HB2	1.92	0.51
1:B:1842:CYS:HA	1:B:1845:ILE:HG22	1.91	0.51
1:C:488:ILE:O	1:C:489:LEU:C	2.51	0.51
1:C:2109:ILE:HG21	1:C:2151:ILE:HB	1.92	0.51
1:B:1224:TRP:CZ3	1:B:1314:ILE:HG13	2.46	0.51
1:A:478:ALA:HB2	1:A:489:LEU:HD12	1.92	0.51
1:A:1224:TRP:CZ3	1:A:1314:ILE:HG13	2.46	0.51
1:B:452:SER:O	1:B:453:LYS:C	2.54	0.51
1:B:2109:ILE:HG21	1:B:2151:ILE:HB	1.92	0.51
1:B:2241:SER:HB2	1:B:2290:LEU:HD12	1.93	0.51
1:C:823:TRP:HE1	1:C:954:ARG:HD2	1.74	0.51
1:C:1151:PHE:HD2	1:C:1152:ILE:H	1.59	0.51
1:B:688:TRP:CZ2	1:B:764:HIS:CB	2.94	0.51
1:B:1250:SER:HB3	1:B:1284:LEU:HD11	1.91	0.51
1:C:688:TRP:CZ2	1:C:764:HIS:CB	2.94	0.51
1:C:2241:SER:HB2	1:C:2290:LEU:HD12	1.93	0.51
1:A:688:TRP:CZ2	1:A:764:HIS:CB	2.94	0.51
1:A:1250:SER:HB3	1:A:1284:LEU:HD11	1.92	0.51
1:A:2061:LEU:CG	1:A:2360:TYR:OH	2.59	0.51
1:B:1215:ARG:HD2	1:B:1218:GLU:HB2	1.91	0.51
1:C:1842:CYS:HA	1:C:1845:ILE:HG22	1.91	0.51
1:A:1351:MET:O	1:A:1352:LYS:C	2.54	0.51
1:B:1351:MET:O	1:B:1352:LYS:C	2.54	0.51
1:B:1687:ARG:HH22	1:B:1711:LEU:HD11	1.76	0.51
1:C:478:ALA:HB2	1:C:489:LEU:HD12	1.92	0.51
1:A:995:TYR:C	1:A:997:PHE:N	2.68	0.50
1:A:1644:TRP:NE1	1:A:1815:ARG:HH12	2.09	0.50
1:B:1826:ARG:HB2	1:B:1826:ARG:NH1	2.25	0.50
1:C:1157:SER:H	1:C:1161:TYR:N	2.10	0.50
1:C:1351:MET:O	1:C:1352:LYS:C	2.54	0.50
1:A:657:PHE:HD2	1:A:728:ILE:HD13	1.76	0.50
1:A:713:TRP:NE1	1:A:717:ASN:HD21	2.09	0.50
1:B:478:ALA:HB2	1:B:489:LEU:HD12	1.92	0.50
1:A:1687:ARG:HH22	1:A:1711:LEU:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ILE:O	1:B:489:LEU:C	2.52	0.50
1:B:631:SER:O	1:B:634:VAL:HB	2.12	0.50
1:B:1822:HIS:CG	1:B:1822:HIS:O	2.65	0.50
1:C:631:SER:O	1:C:634:VAL:HB	2.12	0.50
1:A:630:LEU:O	1:A:634:VAL:HG23	2.11	0.50
1:B:1151:PHE:HD2	1:B:1152:ILE:H	1.59	0.50
1:C:452:SER:O	1:C:453:LYS:C	2.54	0.50
1:C:1826:ARG:NH1	1:C:1826:ARG:HB2	2.25	0.50
1:A:1078:ILE:N	1:A:1079:PRO:HD2	2.27	0.50
1:B:2040:LEU:O	1:B:2041:VAL:C	2.55	0.50
1:C:938:VAL:O	1:C:942:ILE:HG12	2.12	0.50
1:C:1078:ILE:N	1:C:1079:PRO:HD2	2.27	0.50
1:C:1644:TRP:NE1	1:C:1815:ARG:HH12	2.10	0.50
1:C:1687:ARG:HH22	1:C:1711:LEU:HD11	1.76	0.50
1:C:2061:LEU:CG	1:C:2360:TYR:OH	2.59	0.50
1:A:2241:SER:HB2	1:A:2290:LEU:HD12	1.93	0.50
1:B:1982:ILE:HG23	1:B:1983:PRO:HD2	1.93	0.50
1:C:687:PHE:HD2	1:C:764:HIS:CE1	2.30	0.50
1:C:2161:GLU:HG3	1:C:2162:ILE:HG23	1.93	0.50
1:A:938:VAL:O	1:A:942:ILE:HG12	2.12	0.50
1:A:1272:THR:O	1:A:1273:CYS:C	2.53	0.50
1:A:1822:HIS:CG	1:A:1822:HIS:O	2.64	0.50
1:A:1982:ILE:HG23	1:A:1983:PRO:HD2	1.93	0.50
1:A:2040:LEU:O	1:A:2041:VAL:C	2.55	0.50
1:B:687:PHE:HD2	1:B:764:HIS:CE1	2.30	0.50
1:A:690:THR:C	1:A:692:THR:N	2.70	0.50
1:A:1389:PHE:HB3	1:A:1390:GLU:HG3	1.94	0.50
1:A:2047:PHE:HA	1:A:2050:ILE:HD12	1.94	0.50
1:B:1391:PRO:HD2	1:B:1396:HIS:CE1	2.47	0.50
1:B:2196:TYR:CE2	1:B:2198:PRO:HA	2.47	0.50
1:C:526:PHE:O	1:C:528:SER:N	2.45	0.50
1:C:657:PHE:HD2	1:C:728:ILE:HD13	1.76	0.50
1:C:1391:PRO:HD2	1:C:1396:HIS:CE1	2.47	0.50
1:C:1585:MET:HA	1:C:1588:ALA:HB3	1.94	0.50
1:C:1982:ILE:HG23	1:C:1983:PRO:HD2	1.93	0.50
1:A:452:SER:O	1:A:453:LYS:C	2.54	0.50
1:B:483:SER:HB2	1:B:485:PHE:CD1	2.41	0.50
1:B:713:TRP:NE1	1:B:717:ASN:HD21	2.09	0.50
1:B:2074:SER:OG	1:B:2195:PRO:HG3	2.12	0.50
1:C:1224:TRP:CZ3	1:C:1314:ILE:HG13	2.46	0.50
1:C:2040:LEU:O	1:C:2041:VAL:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:PHE:HD2	1:A:764:HIS:CE1	2.30	0.49
1:B:852:PRO:HG2	1:B:878:TYR:CZ	2.47	0.49
1:C:630:LEU:O	1:C:634:VAL:HG23	2.11	0.49
1:A:2373:ARG:HH22	1:B:1986:PHE:HD2	1.55	0.49
1:C:852:PRO:HG2	1:C:878:TYR:CZ	2.47	0.49
1:A:1082:SER:CB	1:A:1249:LEU:HD22	2.43	0.49
1:A:1157:SER:H	1:A:1161:TYR:N	2.10	0.49
1:B:2061:LEU:CG	1:B:2360:TYR:OH	2.59	0.49
1:C:677:PHE:HA	1:C:680:TYR:CD1	2.47	0.49
1:A:526:PHE:O	1:A:528:SER:N	2.45	0.49
1:B:643:SER:HB3	1:B:666:TRP:HH2	1.77	0.49
1:B:677:PHE:HA	1:B:680:TYR:CD1	2.48	0.49
1:B:938:VAL:O	1:B:942:ILE:HG12	2.12	0.49
1:B:1157:SER:H	1:B:1161:TYR:N	2.09	0.49
1:B:1389:PHE:HB3	1:B:1390:GLU:HG3	1.94	0.49
1:C:492:LEU:HD23	1:C:492:LEU:C	2.37	0.49
1:C:2227:ALA:HB2	1:C:2234:HIS:HB3	1.95	0.49
1:A:631:SER:O	1:A:634:VAL:HB	2.12	0.49
1:A:1391:PRO:HD2	1:A:1396:HIS:CE1	2.47	0.49
1:B:1078:ILE:N	1:B:1079:PRO:HD2	2.27	0.49
1:A:492:LEU:HD23	1:A:492:LEU:C	2.37	0.49
1:A:551:LEU:HB2	1:A:554:HIS:HB2	1.94	0.49
1:A:1631:GLY:HA3	1:A:1702:GLY:HA2	1.95	0.49
1:B:526:PHE:O	1:B:528:SER:N	2.45	0.49
1:B:1644:TRP:NE1	1:B:1815:ARG:HH12	2.09	0.49
1:C:1881:MET:O	1:C:1885:ILE:HG12	2.12	0.49
1:A:852:PRO:HG2	1:A:878:TYR:CZ	2.47	0.49
1:B:492:LEU:HD23	1:B:492:LEU:C	2.37	0.49
1:B:2161:GLU:HG3	1:B:2162:ILE:HG23	1.93	0.49
1:C:551:LEU:HB2	1:C:554:HIS:HB2	1.94	0.49
1:C:690:THR:C	1:C:692:THR:N	2.70	0.49
1:C:840:ILE:HD12	1:C:841:PHE:N	2.28	0.49
1:C:1314:ILE:HA	1:C:1317:PHE:CE1	2.48	0.49
1:C:1330:ARG:O	1:C:1332:GLU:N	2.46	0.49
1:C:2074:SER:OG	1:C:2195:PRO:HG3	2.12	0.49
1:A:840:ILE:HD12	1:A:841:PHE:N	2.28	0.49
1:A:1084:ASP:OD2	1:A:1279:HIS:HB2	2.12	0.49
1:A:1330:ARG:O	1:A:1332:GLU:N	2.46	0.49
1:B:690:THR:C	1:B:692:THR:N	2.70	0.49
1:B:1330:ARG:O	1:B:1332:GLU:N	2.45	0.49
1:B:2439:LYS:HA	1:B:2442:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:ASP:O	1:C:984:SER:N	2.46	0.49
1:A:643:SER:HB3	1:A:666:TRP:HH2	1.77	0.49
1:A:1179:LEU:HD21	1:A:1227:LEU:HD21	1.95	0.49
1:A:2074:SER:OG	1:A:2195:PRO:HG3	2.12	0.49
1:B:840:ILE:HD12	1:B:841:PHE:N	2.28	0.49
1:C:1179:LEU:HD21	1:C:1227:LEU:HD21	1.95	0.49
1:C:2196:TYR:CE2	1:C:2198:PRO:HA	2.47	0.49
1:A:1881:MET:O	1:A:1885:ILE:HG12	2.12	0.49
1:A:2196:TYR:CE2	1:A:2198:PRO:HA	2.47	0.49
1:A:1314:ILE:HA	1:A:1317:PHE:CE1	2.48	0.48
1:B:982:ASP:O	1:B:984:SER:N	2.46	0.48
1:B:1380:ILE:CD1	1:B:1405:MET:HA	2.33	0.48
1:C:643:SER:HB3	1:C:666:TRP:HH2	1.77	0.48
1:C:1389:PHE:HB3	1:C:1390:GLU:HG3	1.94	0.48
1:C:1631:GLY:HA3	1:C:1702:GLY:HA2	1.95	0.48
1:A:484:ILE:HD13	1:A:544:VAL:HG23	1.96	0.48
1:C:1084:ASP:OD2	1:C:1279:HIS:HB2	2.12	0.48
1:A:995:TYR:O	1:A:996:GLY:C	2.56	0.48
1:B:995:TYR:O	1:B:996:GLY:C	2.56	0.48
1:B:1585:MET:HA	1:B:1588:ALA:HB3	1.94	0.48
1:B:1084:ASP:OD2	1:B:1279:HIS:HB2	2.12	0.48
1:B:1211:ASN:HA	1:B:1326:MET:HE1	1.96	0.48
1:B:1240:CYS:O	1:B:1243:ILE:HG22	2.13	0.48
1:B:1881:MET:O	1:B:1885:ILE:HG12	2.12	0.48
1:C:1082:SER:CB	1:C:1249:LEU:HD22	2.43	0.48
1:C:1240:CYS:O	1:C:1243:ILE:HG22	2.13	0.48
1:A:982:ASP:O	1:A:984:SER:N	2.46	0.48
1:A:1211:ASN:HA	1:A:1326:MET:HE1	1.96	0.48
1:A:2161:GLU:HG3	1:A:2162:ILE:HG23	1.93	0.48
1:B:551:LEU:HB2	1:B:554:HIS:HB2	1.94	0.48
1:B:1382:ARG:C	1:B:1384:ALA:N	2.70	0.48
1:B:2047:PHE:HA	1:B:2050:ILE:HD12	1.94	0.48
1:C:484:ILE:HD13	1:C:544:VAL:HG23	1.96	0.48
1:C:1005:THR:HG22	1:C:1009:ILE:HD11	1.95	0.48
1:A:677:PHE:HA	1:A:680:TYR:CD1	2.48	0.48
1:A:692:THR:HB	1:A:753:PHE:HE1	1.79	0.48
1:A:2353:LYS:O	1:A:2357:ILE:HG12	2.14	0.48
1:B:692:THR:HB	1:B:753:PHE:HE1	1.79	0.48
1:B:1095:LEU:CD2	1:B:1096:SER:H	2.27	0.48
1:A:1585:MET:HA	1:A:1588:ALA:HB3	1.94	0.48
1:B:2196:TYR:O	1:B:2196:TYR:CD1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:LEU:HD13	1:A:882:VAL:CB	2.42	0.48
1:A:1240:CYS:O	1:A:1243:ILE:HG22	2.13	0.48
1:B:1082:SER:HB3	1:B:1249:LEU:HD13	1.95	0.48
1:C:1211:ASN:HA	1:C:1326:MET:HE1	1.96	0.48
1:C:1828:ILE:N	1:C:1828:ILE:HD12	2.29	0.48
1:C:2047:PHE:HA	1:C:2050:ILE:HD12	1.94	0.48
1:C:2196:TYR:CD1	1:C:2196:TYR:O	2.67	0.48
1:A:526:PHE:C	1:A:528:SER:N	2.72	0.48
1:A:2439:LYS:HA	1:A:2442:GLU:HB3	1.95	0.48
1:B:995:TYR:C	1:B:997:PHE:N	2.68	0.48
1:B:1631:GLY:HA3	1:B:1702:GLY:HA2	1.95	0.48
1:C:1822:HIS:CG	1:C:1822:HIS:O	2.65	0.48
1:B:2197:ASP:HA	1:B:2198:PRO:HD2	1.68	0.48
1:A:1178:THR:HB	1:A:1306:ALA:HA	1.96	0.47
1:B:2353:LYS:O	1:B:2357:ILE:HG12	2.14	0.47
1:C:526:PHE:C	1:C:528:SER:N	2.72	0.47
1:C:692:THR:HB	1:C:753:PHE:HE1	1.79	0.47
1:C:995:TYR:O	1:C:996:GLY:C	2.56	0.47
1:A:1082:SER:HB3	1:A:1249:LEU:HD13	1.95	0.47
1:A:2352:PHE:CE2	1:A:2355:GLY:N	2.82	0.47
1:B:2352:PHE:CE2	1:B:2355:GLY:N	2.82	0.47
1:C:1178:THR:HB	1:C:1306:ALA:HA	1.96	0.47
1:C:2353:LYS:O	1:C:2357:ILE:HG12	2.14	0.47
1:A:483:SER:HB2	1:A:485:PHE:CD1	2.41	0.47
1:A:1005:THR:HG22	1:A:1009:ILE:HD11	1.95	0.47
1:A:1828:ILE:HD12	1:A:1828:ILE:N	2.29	0.47
1:A:2196:TYR:O	1:A:2196:TYR:CD1	2.67	0.47
1:A:2227:ALA:HB2	1:A:2234:HIS:HB3	1.95	0.47
1:B:1207:LEU:HD11	1:B:1219:HIS:ND1	2.24	0.47
1:C:225:THR:HA	1:C:577:ARG:CG	2.38	0.47
1:C:1095:LEU:CD2	1:C:1096:SER:H	2.27	0.47
1:A:1095:LEU:CD2	1:A:1096:SER:H	2.27	0.47
1:B:484:ILE:HD13	1:B:544:VAL:HG23	1.96	0.47
1:B:1179:LEU:HD21	1:B:1227:LEU:HD21	1.95	0.47
1:C:2352:PHE:CE2	1:C:2355:GLY:N	2.82	0.47
1:A:1151:PHE:HD2	1:A:1152:ILE:H	1.59	0.47
1:C:995:TYR:C	1:C:997:PHE:N	2.68	0.47
1:C:1082:SER:HB3	1:C:1249:LEU:HD13	1.95	0.47
1:C:2439:LYS:HA	1:C:2442:GLU:HB3	1.95	0.47
1:A:1375:ARG:NH2	1:A:1379:GLN:OE1	2.48	0.47
1:B:565:LEU:HD23	1:B:565:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2078:LYS:HB3	1:A:2193:THR:HB	1.97	0.47
1:B:849:LEU:HD13	1:B:882:VAL:CB	2.42	0.47
1:B:1252:PHE:CE1	1:B:1262:LEU:HB3	2.50	0.47
1:B:2227:ALA:HB2	1:B:2234:HIS:HB3	1.95	0.47
1:C:478:ALA:HB2	1:C:489:LEU:CD1	2.45	0.47
1:C:565:LEU:O	1:C:565:LEU:HD23	2.14	0.47
1:A:565:LEU:HD23	1:A:565:LEU:O	2.14	0.47
1:B:1191:LEU:HB2	1:B:1672:PHE:CE2	2.50	0.47
1:B:2431:ILE:HG12	1:C:2425:ARG:CZ	2.45	0.47
1:A:1382:ARG:C	1:A:1384:ALA:N	2.70	0.47
1:B:939:ILE:HD12	1:B:940:VAL:N	2.30	0.47
1:B:1314:ILE:HA	1:B:1317:PHE:CE1	2.48	0.47
1:C:1685:THR:O	1:C:1689:GLU:HG2	2.15	0.47
1:A:686:ALA:C	1:A:688:TRP:N	2.73	0.47
1:A:1252:PHE:CE1	1:A:1262:LEU:HB3	2.50	0.47
1:B:526:PHE:C	1:B:528:SER:N	2.72	0.47
1:C:1382:ARG:C	1:C:1384:ALA:N	2.70	0.47
1:A:688:TRP:CD1	1:A:760:LEU:HG	2.50	0.46
1:A:2271:ARG:HA	1:A:2271:ARG:HD3	1.62	0.46
1:A:2431:ILE:HG12	1:B:2425:ARG:CZ	2.45	0.46
1:B:636:VAL:HG12	1:B:637:TYR:CD1	2.51	0.46
1:A:1986:PHE:HD2	1:C:2373:ARG:HH22	1.55	0.46
1:B:1005:THR:HG22	1:B:1009:ILE:HD11	1.95	0.46
1:B:1685:THR:O	1:B:1689:GLU:HG2	2.15	0.46
1:B:2064:TRP:HD1	1:C:1871:PRO:HG3	1.69	0.46
1:C:636:VAL:HG12	1:C:637:TYR:CD1	2.50	0.46
1:C:939:ILE:HD12	1:C:940:VAL:N	2.30	0.46
1:A:636:VAL:HG12	1:A:637:TYR:CD1	2.51	0.46
1:A:1241:LEU:HD23	1:A:1241:LEU:HA	1.81	0.46
1:B:1271:ILE:HG13	1:B:1293:VAL:HG13	1.98	0.46
1:C:1826:ARG:HB2	1:C:1826:ARG:HH11	1.80	0.46
1:C:2078:LYS:HB3	1:C:2193:THR:HB	1.97	0.46
1:A:990:GLN:C	1:A:992:LEU:N	2.73	0.46
1:A:1646:ASN:ND2	1:A:1945:LEU:HD23	2.31	0.46
1:A:2197:ASP:HA	1:A:2198:PRO:HD2	1.68	0.46
1:B:1346:LEU:O	1:B:1350:GLU:HG2	2.15	0.46
1:B:1826:ARG:HB2	1:B:1826:ARG:HH11	1.80	0.46
1:C:1252:PHE:CE1	1:C:1262:LEU:HB3	2.50	0.46
1:A:1271:ILE:HG13	1:A:1293:VAL:HG13	1.98	0.46
1:A:1846:MET:HE3	1:A:1846:MET:HB2	1.71	0.46
1:A:2196:TYR:O	1:A:2196:TYR:CG	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:ILE:O	1:B:1056:LEU:HD22	2.16	0.46
1:C:483:SER:HB2	1:C:485:PHE:CD1	2.41	0.46
1:A:986:LYS:HA	1:A:989:ILE:HB	1.98	0.46
1:A:1826:ARG:HB2	1:A:1826:ARG:HH11	1.80	0.46
1:B:478:ALA:HB2	1:B:489:LEU:CD1	2.45	0.46
1:B:1375:ARG:NH2	1:B:1379:GLN:OE1	2.48	0.46
1:C:688:TRP:CD1	1:C:760:LEU:HG	2.50	0.46
1:C:1052:ILE:O	1:C:1056:LEU:HD22	2.16	0.46
1:C:1346:LEU:O	1:C:1350:GLU:HG2	2.15	0.46
1:A:1346:LEU:O	1:A:1350:GLU:HG2	2.15	0.46
1:B:1646:ASN:ND2	1:B:1945:LEU:HD23	2.31	0.46
1:C:1191:LEU:HB2	1:C:1672:PHE:CE2	2.50	0.46
1:A:494:CYS:HA	1:A:497:TRP:CD1	2.49	0.46
1:B:484:ILE:O	1:B:487:LEU:HB3	2.16	0.46
1:B:1584:LYS:HD2	1:B:1584:LYS:HA	1.74	0.46
1:A:1342:LEU:O	1:A:1343:LYS:C	2.59	0.46
1:A:1380:ILE:CD1	1:A:1405:MET:HA	2.33	0.46
1:A:1693:ASP:HA	1:A:1694:PRO:HD3	1.84	0.46
1:A:1904:GLN:NE2	1:A:1951:ILE:HD12	2.31	0.46
1:B:225:THR:HA	1:B:577:ARG:CG	2.38	0.46
1:B:688:TRP:CD1	1:B:760:LEU:HG	2.51	0.46
1:B:1828:ILE:HD12	1:B:1828:ILE:N	2.29	0.46
1:A:1052:ILE:O	1:A:1056:LEU:HD22	2.16	0.46
1:A:1685:THR:O	1:A:1689:GLU:HG2	2.15	0.46
1:A:2064:TRP:CD1	1:B:1871:PRO:CG	2.89	0.46
1:A:2425:ARG:CZ	1:C:2431:ILE:HG12	2.45	0.46
1:B:986:LYS:HA	1:B:989:ILE:HB	1.98	0.46
1:C:1375:ARG:NH2	1:C:1379:GLN:OE1	2.48	0.46
1:C:1828:ILE:N	1:C:1828:ILE:CD1	2.80	0.46
1:A:484:ILE:O	1:A:487:LEU:HB3	2.16	0.45
1:A:814:LEU:O	1:A:818:THR:HG23	2.17	0.45
1:B:1178:THR:HB	1:B:1306:ALA:HA	1.96	0.45
1:C:471:LEU:O	1:C:475:MET:HG2	2.17	0.45
1:A:1217:PHE:O	1:A:1220:THR:HG22	2.16	0.45
1:B:1269:PHE:O	1:B:1271:ILE:HG22	2.16	0.45
1:C:1158:TYR:CZ	1:C:1600:THR:HG21	2.52	0.45
1:C:1342:LEU:O	1:C:1343:LYS:C	2.59	0.45
1:C:2178:LEU:HD23	1:C:2184:VAL:HG21	1.98	0.45
1:A:939:ILE:HD12	1:A:940:VAL:N	2.30	0.45
1:A:1013:ILE:HD12	1:A:1013:ILE:HA	1.82	0.45
1:A:1191:LEU:HB2	1:A:1672:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:ILE:HG12	1:A:1293:VAL:HG13	1.99	0.45
1:B:2078:LYS:HB3	1:B:2193:THR:HB	1.97	0.45
1:C:1224:TRP:CH2	1:C:1314:ILE:HG13	2.52	0.45
1:C:1269:PHE:O	1:C:1271:ILE:HG22	2.16	0.45
1:C:1904:GLN:NE2	1:C:1951:ILE:HD12	2.31	0.45
1:A:809:LYS:HB3	1:A:809:LYS:HE3	1.73	0.45
1:A:1044:VAL:HG13	1:A:1121:LEU:HD21	1.99	0.45
1:A:1149:TYR:HB3	1:A:1320:TRP:CZ3	2.52	0.45
1:A:1828:ILE:N	1:A:1828:ILE:CD1	2.80	0.45
1:B:471:LEU:O	1:B:475:MET:HG2	2.17	0.45
1:B:1082:SER:CB	1:B:1249:LEU:HD22	2.43	0.45
1:B:1149:TYR:HB3	1:B:1320:TRP:CZ3	2.51	0.45
1:B:1904:GLN:NE2	1:B:1951:ILE:HD12	2.31	0.45
1:C:1646:ASN:ND2	1:C:1945:LEU:HD23	2.31	0.45
1:C:1711:LEU:HB3	1:C:1712:TRP:H	1.55	0.45
1:A:1005:THR:HG22	1:A:1009:ILE:CD1	2.47	0.45
1:A:1641:SER:HA	1:A:1656:PHE:CZ	2.49	0.45
1:B:1342:LEU:O	1:B:1343:LYS:C	2.59	0.45
1:C:483:SER:HG	1:C:486:GLY:N	2.13	0.45
1:C:849:LEU:HD13	1:C:882:VAL:CB	2.42	0.45
1:B:1217:PHE:O	1:B:1220:THR:HG22	2.17	0.45
1:C:760:LEU:HA	1:C:764:HIS:CE1	2.52	0.45
1:C:1005:THR:HG22	1:C:1009:ILE:CD1	2.47	0.45
1:C:1149:TYR:HB3	1:C:1320:TRP:CZ3	2.51	0.45
1:C:484:ILE:O	1:C:487:LEU:HB3	2.16	0.45
1:C:516:TYR:CD1	1:C:519:PHE:HE2	2.35	0.45
1:C:1380:ILE:HD12	1:C:1405:MET:CA	2.35	0.45
1:A:471:LEU:O	1:A:475:MET:HG2	2.17	0.45
1:A:478:ALA:HB2	1:A:489:LEU:CD1	2.45	0.45
1:A:516:TYR:CD1	1:A:519:PHE:HE2	2.35	0.45
1:A:760:LEU:HD12	1:A:764:HIS:CE1	2.52	0.45
1:A:991:PHE:HB3	1:A:995:TYR:HB2	1.99	0.45
1:A:1158:TYR:CZ	1:A:1600:THR:HG21	2.52	0.45
1:A:1224:TRP:CH2	1:A:1314:ILE:HG13	2.52	0.45
1:B:814:LEU:O	1:B:818:THR:HG23	2.17	0.45
1:B:942:ILE:O	1:B:945:LEU:HD23	2.17	0.45
1:B:978:HIS:O	1:B:981:PHE:HB3	2.17	0.45
1:B:2064:TRP:CD1	1:C:1871:PRO:CG	2.89	0.45
1:C:986:LYS:HA	1:C:989:ILE:HB	1.98	0.45
1:A:1269:PHE:O	1:A:1271:ILE:HG22	2.16	0.45
1:B:494:CYS:HA	1:B:497:TRP:CD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:TYR:CZ	1:B:1600:THR:HG21	2.52	0.45
1:C:939:ILE:HA	1:C:942:ILE:HG12	1.99	0.45
1:C:1378:LYS:O	1:C:1379:GLN:C	2.60	0.45
1:C:1825:PHE:CD2	1:C:1825:PHE:O	2.70	0.45
1:A:939:ILE:HA	1:A:942:ILE:HG12	1.99	0.45
1:A:1825:PHE:CD2	1:A:1825:PHE:O	2.70	0.45
1:A:1900:LYS:NZ	1:A:1900:LYS:HB3	2.32	0.45
1:B:990:GLN:C	1:B:992:LEU:N	2.73	0.45
1:B:1176:MET:CE	1:B:1179:LEU:HD22	2.36	0.45
1:B:1378:LYS:O	1:B:1379:GLN:C	2.60	0.45
1:B:1828:ILE:N	1:B:1828:ILE:CD1	2.80	0.45
1:B:760:LEU:HD12	1:B:764:HIS:CE1	2.52	0.44
1:B:854:VAL:O	1:B:857:LEU:HB3	2.17	0.44
1:B:2178:LEU:HD23	1:B:2184:VAL:HG21	1.98	0.44
1:C:814:LEU:O	1:C:818:THR:HG23	2.17	0.44
1:C:942:ILE:O	1:C:945:LEU:HD23	2.17	0.44
1:C:1149:TYR:HB2	1:C:1319:SER:OG	2.17	0.44
1:C:1217:PHE:O	1:C:1220:THR:HG22	2.16	0.44
1:C:1271:ILE:HG13	1:C:1293:VAL:HG13	1.98	0.44
1:C:1367:ARG:O	1:C:1371:ALA:N	2.49	0.44
1:C:2365:LEU:O	1:C:2366:VAL:C	2.60	0.44
1:A:807:LEU:O	1:A:807:LEU:HD12	2.17	0.44
1:A:2365:LEU:O	1:A:2366:VAL:C	2.60	0.44
1:B:760:LEU:HA	1:B:764:HIS:CE1	2.52	0.44
1:B:939:ILE:HA	1:B:942:ILE:HG12	1.99	0.44
1:B:1005:THR:HG22	1:B:1009:ILE:CD1	2.47	0.44
1:B:1825:PHE:O	1:B:1825:PHE:CD2	2.70	0.44
1:C:483:SER:C	1:C:486:GLY:N	2.74	0.44
1:C:523:LEU:HA	1:C:526:PHE:CD2	2.52	0.44
1:C:1044:VAL:HG13	1:C:1121:LEU:HD21	1.99	0.44
1:C:1900:LYS:NZ	1:C:1900:LYS:HB3	2.32	0.44
1:C:2052:GLY:O	1:C:2055:ILE:HG13	2.17	0.44
1:A:483:SER:OG	1:A:485:PHE:HB2	2.18	0.44
1:A:942:ILE:O	1:A:945:LEU:HD23	2.17	0.44
1:B:1013:ILE:HD12	1:B:1021:ALA:HB1	2.00	0.44
1:B:1159:VAL:HG23	1:B:1160:ASP:H	1.83	0.44
1:B:1224:TRP:CH2	1:B:1314:ILE:HG13	2.52	0.44
1:B:1641:SER:HA	1:B:1656:PHE:CZ	2.49	0.44
1:C:760:LEU:HD12	1:C:764:HIS:CE1	2.52	0.44
1:C:833:ILE:HG22	1:C:837:ILE:HD13	1.99	0.44
1:C:1240:CYS:HA	1:C:1243:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:C	1:A:490:LEU:CD2	2.91	0.44
1:A:978:HIS:O	1:A:981:PHE:HB3	2.17	0.44
1:A:1155:LYS:O	1:A:1156:LYS:HB2	2.17	0.44
1:A:1378:LYS:O	1:A:1379:GLN:C	2.60	0.44
1:A:2368:GLY:HA2	1:A:2372:VAL:HB	1.99	0.44
1:A:2378:THR:HG1	1:B:2008:ASN:CG	2.23	0.44
1:B:523:LEU:HA	1:B:526:PHE:CD2	2.52	0.44
1:B:1237:MET:HA	1:B:1240:CYS:SG	2.57	0.44
1:B:1900:LYS:NZ	1:B:1900:LYS:HB3	2.32	0.44
1:B:2196:TYR:O	1:B:2196:TYR:CG	2.68	0.44
1:B:2368:GLY:HA2	1:B:2372:VAL:HB	1.99	0.44
1:C:1221:LEU:HA	1:C:1224:TRP:CD1	2.53	0.44
1:A:523:LEU:HA	1:A:526:PHE:CD2	2.52	0.44
1:A:1237:MET:HA	1:A:1240:CYS:SG	2.57	0.44
1:A:2052:GLY:O	1:A:2055:ILE:HG13	2.17	0.44
1:B:639:ILE:O	1:B:643:SER:OG	2.35	0.44
1:B:807:LEU:HD12	1:B:807:LEU:O	2.17	0.44
1:B:981:PHE:O	1:B:982:ASP:C	2.60	0.44
1:B:1149:TYR:HB2	1:B:1319:SER:OG	2.17	0.44
1:B:1838:ILE:HG23	1:B:1939:ILE:HG23	2.00	0.44
1:C:483:SER:OG	1:C:485:PHE:HB2	2.18	0.44
1:C:807:LEU:HD12	1:C:807:LEU:O	2.17	0.44
1:C:978:HIS:O	1:C:981:PHE:HB3	2.17	0.44
1:A:981:PHE:O	1:A:982:ASP:C	2.60	0.44
1:A:1240:CYS:HA	1:A:1243:ILE:HG22	1.98	0.44
1:A:1347:ILE:O	1:A:1351:MET:HG2	2.17	0.44
1:B:939:ILE:HD12	1:B:940:VAL:H	1.82	0.44
1:B:1044:VAL:HG13	1:B:1121:LEU:HD21	1.99	0.44
1:B:1240:CYS:HA	1:B:1243:ILE:HG22	1.98	0.44
1:C:854:VAL:O	1:C:857:LEU:HB3	2.17	0.44
1:C:1237:MET:HA	1:C:1240:CYS:SG	2.57	0.44
1:C:1317:PHE:HB2	1:C:1322:PHE:CD1	2.53	0.44
1:A:519:PHE:HA	1:A:522:ILE:HD12	2.00	0.44
1:A:1149:TYR:HB2	1:A:1319:SER:OG	2.17	0.44
1:B:516:TYR:CD1	1:B:519:PHE:HE2	2.35	0.44
1:B:981:PHE:CG	1:B:982:ASP:N	2.85	0.44
1:B:1347:ILE:O	1:B:1351:MET:HG2	2.17	0.44
1:B:1367:ARG:O	1:B:1371:ALA:N	2.49	0.44
1:B:2052:GLY:O	1:B:2055:ILE:HG13	2.17	0.44
1:B:2365:LEU:O	1:B:2366:VAL:C	2.60	0.44
1:B:2373:ARG:HH22	1:C:1986:PHE:HD2	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:GLN:C	1:C:992:LEU:N	2.73	0.44
1:A:679:LEU:HD13	1:A:679:LEU:HA	1.85	0.44
1:A:1159:VAL:HG23	1:A:1160:ASP:H	1.83	0.44
1:A:1317:PHE:HB2	1:A:1322:PHE:CD1	2.53	0.44
1:A:2178:LEU:HD23	1:A:2184:VAL:HG21	1.98	0.44
1:A:2272:ILE:HD13	1:A:2272:ILE:HA	1.80	0.44
1:B:1000:PHE:HB3	1:B:1001:GLY:H	1.32	0.44
1:B:1228:LEU:O	1:B:1232:LEU:HD13	2.18	0.44
1:C:939:ILE:HD12	1:C:940:VAL:H	1.82	0.44
1:C:1271:ILE:HG12	1:C:1293:VAL:HG13	1.99	0.44
1:C:1937:TYR:HD1	1:C:1937:TYR:O	2.01	0.44
1:A:1221:LEU:HA	1:A:1224:TRP:CD1	2.53	0.44
1:B:307:TRP:O	1:B:311:ALA:HB2	2.18	0.44
1:B:529:MET:O	1:B:531:ILE:N	2.49	0.44
1:C:686:ALA:C	1:C:688:TRP:N	2.73	0.44
1:C:1187:SER:O	1:C:1190:ALA:HB3	2.18	0.44
1:C:1870:ILE:HG23	1:C:1871:PRO:HD2	2.00	0.44
1:C:1940:LYS:HD2	1:C:1940:LYS:HA	1.76	0.44
1:C:2076:PRO:HG3	1:C:2194:ARG:HE	1.83	0.44
1:C:2298:LYS:HB3	1:C:2298:LYS:HE2	1.83	0.44
1:A:981:PHE:CG	1:A:982:ASP:N	2.86	0.43
1:A:2076:PRO:HG3	1:A:2194:ARG:NE	2.33	0.43
1:B:519:PHE:HA	1:B:522:ILE:HD12	2.00	0.43
1:B:833:ILE:HG22	1:B:837:ILE:HD13	1.99	0.43
1:B:833:ILE:O	1:B:837:ILE:HG12	2.18	0.43
1:B:1589:VAL:HB	1:B:1593:TRP:NE1	2.33	0.43
1:B:1846:MET:HE3	1:B:1846:MET:HB2	1.71	0.43
1:C:490:LEU:C	1:C:490:LEU:CD2	2.91	0.43
1:C:1013:ILE:HD12	1:C:1021:ALA:HB1	2.00	0.43
1:C:1043:TRP:HA	1:C:1046:TYR:HB3	2.00	0.43
1:A:760:LEU:HA	1:A:764:HIS:CE1	2.52	0.43
1:A:1584:LYS:HD2	1:A:1584:LYS:HA	1.74	0.43
1:A:1838:ILE:HG23	1:A:1939:ILE:HG23	2.00	0.43
1:A:1871:PRO:CG	1:C:2064:TRP:CD1	2.89	0.43
1:A:2076:PRO:HG3	1:A:2194:ARG:HE	1.83	0.43
1:B:483:SER:OG	1:B:485:PHE:HB2	2.18	0.43
1:B:696:SER:O	1:B:700:ILE:HG23	2.18	0.43
1:B:1187:SER:O	1:B:1190:ALA:HB3	2.18	0.43
1:B:1221:LEU:HA	1:B:1224:TRP:CD1	2.53	0.43
1:C:833:ILE:O	1:C:837:ILE:HG12	2.18	0.43
1:A:696:SER:O	1:A:700:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:VAL:O	1:A:857:LEU:HB3	2.17	0.43
1:A:939:ILE:HD12	1:A:940:VAL:H	1.82	0.43
1:A:1065:PRO:HB2	1:A:1066:PRO:HD3	2.00	0.43
1:A:1589:VAL:HB	1:A:1593:TRP:NE1	2.33	0.43
1:B:828:VAL:HG12	1:B:829:HIS:CG	2.53	0.43
1:B:991:PHE:HB3	1:B:995:TYR:HB2	1.99	0.43
1:B:1180:ALA:HA	1:B:1183:ILE:HD12	2.01	0.43
1:C:638:PHE:CB	1:C:763:PHE:CZ	2.99	0.43
1:C:1036:ARG:O	1:C:1040:ARG:HG3	2.19	0.43
1:C:1838:ILE:HG23	1:C:1939:ILE:HG23	2.00	0.43
1:A:1013:ILE:HD12	1:A:1021:ALA:HB1	2.00	0.43
1:A:1228:LEU:O	1:A:1232:LEU:HD13	2.18	0.43
1:B:1155:LYS:O	1:B:1156:LYS:HB2	2.17	0.43
1:B:1634:THR:O	1:B:1638:PRO:HD2	2.18	0.43
1:B:2076:PRO:HG3	1:B:2194:ARG:NE	2.33	0.43
1:B:2076:PRO:HG3	1:B:2194:ARG:HE	1.83	0.43
1:C:2368:GLY:HA2	1:C:2372:VAL:HB	1.99	0.43
1:A:202:ILE:HA	1:A:559:LEU:HD23	2.00	0.43
1:A:833:ILE:O	1:A:837:ILE:HG12	2.18	0.43
1:A:2363:VAL:HG13	1:A:2364:ILE:N	2.33	0.43
1:B:994:ASP:C	1:B:996:GLY:H	2.26	0.43
1:B:1047:VAL:HG21	1:B:1121:LEU:HG	2.01	0.43
1:B:1241:LEU:HD23	1:B:1241:LEU:HA	1.81	0.43
1:B:1271:ILE:HG12	1:B:1293:VAL:HG13	1.99	0.43
1:B:1317:PHE:HB2	1:B:1322:PHE:CD1	2.53	0.43
1:B:2271:ARG:HD3	1:B:2271:ARG:HA	1.62	0.43
1:C:981:PHE:O	1:C:982:ASP:C	2.60	0.43
1:C:1159:VAL:HG23	1:C:1160:ASP:H	1.83	0.43
1:C:2384:MET:H	1:C:2384:MET:HG2	1.57	0.43
1:B:1249:LEU:HD21	1:B:1281:LEU:CD2	2.48	0.43
1:B:1937:TYR:HD1	1:B:1937:TYR:O	2.01	0.43
1:C:981:PHE:CG	1:C:982:ASP:N	2.86	0.43
1:C:991:PHE:HB3	1:C:995:TYR:HB2	1.99	0.43
1:C:1628:MET:HE3	1:C:1718:PHE:CE2	2.54	0.43
1:C:2076:PRO:HG3	1:C:2194:ARG:NE	2.33	0.43
1:C:2363:VAL:HG13	1:C:2364:ILE:N	2.33	0.43
1:A:638:PHE:CB	1:A:763:PHE:CZ	2.99	0.43
1:A:828:VAL:HG12	1:A:829:HIS:CG	2.53	0.43
1:A:833:ILE:HG22	1:A:837:ILE:HD13	2.00	0.43
1:B:1043:TRP:HA	1:B:1046:TYR:HB3	2.00	0.43
1:B:1700:LEU:HD23	1:B:1700:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:SER:O	1:C:700:ILE:HG23	2.18	0.43
1:C:1056:LEU:HA	1:C:1059:PHE:HB2	2.01	0.43
1:C:1155:LYS:O	1:C:1156:LYS:HB2	2.17	0.43
1:C:1228:LEU:O	1:C:1232:LEU:HD13	2.18	0.43
1:C:1347:ILE:O	1:C:1351:MET:HG2	2.17	0.43
1:A:653:PHE:CG	1:A:654:ALA:N	2.87	0.43
1:A:1344:ASN:HA	1:A:1347:ILE:HG22	2.01	0.43
1:A:1634:THR:O	1:A:1638:PRO:HD2	2.18	0.43
1:B:2020:LYS:HB2	1:B:2391:ALA:O	2.19	0.43
1:B:2363:VAL:HG13	1:B:2364:ILE:N	2.33	0.43
1:C:307:TRP:O	1:C:311:ALA:HB2	2.18	0.43
1:C:487:LEU:HD13	1:C:703:TYR:HD2	1.84	0.43
1:C:653:PHE:CG	1:C:654:ALA:N	2.87	0.43
1:C:994:ASP:C	1:C:996:GLY:H	2.26	0.43
1:C:1325:CYS:HA	1:C:1328:GLU:HB2	2.00	0.43
1:C:2020:LYS:HB2	1:C:2391:ALA:O	2.19	0.43
1:C:2196:TYR:O	1:C:2196:TYR:CG	2.68	0.43
1:C:2245:PHE:HB3	1:C:2339:PHE:HE2	1.83	0.43
1:A:1187:SER:O	1:A:1190:ALA:HB3	2.18	0.43
1:A:1243:ILE:O	1:A:1247:VAL:HG13	2.19	0.43
1:A:1870:ILE:HG23	1:A:1871:PRO:HD2	2.00	0.43
1:B:2245:PHE:HB3	1:B:2339:PHE:HE2	1.83	0.43
1:C:1020:LEU:HD13	1:C:1024:GLN:HE22	1.84	0.43
1:C:1241:LEU:HD23	1:C:1241:LEU:HA	1.81	0.43
1:A:487:LEU:HD13	1:A:703:TYR:HD2	1.84	0.43
1:B:487:LEU:HD13	1:B:703:TYR:HD2	1.84	0.43
1:B:1628:MET:HE3	1:B:1718:PHE:CE2	2.54	0.43
1:B:2298:LYS:HE2	1:B:2298:LYS:HB3	1.83	0.43
1:C:494:CYS:HA	1:C:497:TRP:CD1	2.49	0.43
1:C:519:PHE:HA	1:C:522:ILE:HD12	2.00	0.43
1:C:826:PHE:O	1:C:830:ILE:HG12	2.19	0.43
1:C:1065:PRO:HB2	1:C:1066:PRO:HD3	2.00	0.43
1:C:1589:VAL:HB	1:C:1593:TRP:NE1	2.33	0.43
1:A:676:SER:O	1:A:679:LEU:HB2	2.19	0.42
1:A:826:PHE:O	1:A:830:ILE:HG12	2.19	0.42
1:A:1349:LYS:O	1:A:1352:LYS:HB3	2.19	0.42
1:A:1686:TRP:CH2	1:A:1698:ASP:CB	3.02	0.42
1:B:989:ILE:O	1:B:992:LEU:HB3	2.19	0.42
1:B:1020:LEU:HD13	1:B:1024:GLN:HE22	1.84	0.42
1:B:1243:ILE:O	1:B:1247:VAL:HG13	2.19	0.42
1:C:454:GLY:O	1:C:455:MET:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:GLY:O	1:C:1002:LEU:C	2.62	0.42
1:C:1047:VAL:HG21	1:C:1121:LEU:HG	2.01	0.42
1:C:1381:GLU:O	1:C:1381:GLU:HG2	2.18	0.42
1:C:1634:THR:O	1:C:1638:PRO:HD2	2.19	0.42
1:A:1047:VAL:HG21	1:A:1121:LEU:HG	2.01	0.42
1:A:1325:CYS:HA	1:A:1328:GLU:HB2	2.00	0.42
1:A:1700:LEU:C	1:A:1700:LEU:HD23	2.44	0.42
1:A:2106:LEU:HD11	1:A:2152:LEU:HD21	2.01	0.42
1:A:2123:ASP:OD1	1:A:2123:ASP:C	2.63	0.42
1:B:653:PHE:CG	1:B:654:ALA:N	2.87	0.42
1:B:1344:ASN:HA	1:B:1347:ILE:HG22	2.01	0.42
1:B:1870:ILE:HG23	1:B:1871:PRO:HD2	2.00	0.42
1:B:2106:LEU:HD11	1:B:2152:LEU:HD21	2.01	0.42
1:C:1243:ILE:O	1:C:1247:VAL:HG13	2.19	0.42
1:C:1700:LEU:C	1:C:1700:LEU:HD23	2.44	0.42
1:B:202:ILE:HA	1:B:559:LEU:HD23	2.00	0.42
1:B:494:CYS:CA	1:B:497:TRP:HD1	2.32	0.42
1:B:1325:CYS:HA	1:B:1328:GLU:HB2	2.00	0.42
1:C:202:ILE:HA	1:C:559:LEU:HD23	2.00	0.42
1:C:676:SER:O	1:C:679:LEU:HB2	2.19	0.42
1:C:828:VAL:HG12	1:C:829:HIS:CG	2.53	0.42
1:A:307:TRP:O	1:A:311:ALA:HB2	2.18	0.42
1:A:1036:ARG:O	1:A:1040:ARG:HG3	2.19	0.42
1:A:1043:TRP:HA	1:A:1046:TYR:HB3	2.00	0.42
1:A:1180:ALA:HA	1:A:1183:ILE:HD12	2.01	0.42
1:A:1916:PHE:CE2	1:A:1937:TYR:HE2	2.37	0.42
1:A:1937:TYR:HD1	1:A:1937:TYR:O	2.01	0.42
1:A:2020:LYS:HB2	1:A:2391:ALA:O	2.19	0.42
1:B:1036:ARG:O	1:B:1040:ARG:HG3	2.19	0.42
1:B:1711:LEU:HB3	1:B:1712:TRP:H	1.55	0.42
1:B:2303:LYS:HE3	1:B:2303:LYS:HB2	1.74	0.42
1:C:875:MET:O	1:C:879:LEU:HG	2.20	0.42
1:C:1378:LYS:HD2	1:C:1382:ARG:NH1	2.35	0.42
1:A:989:ILE:O	1:A:992:LEU:HB3	2.19	0.42
1:A:1378:LYS:HD2	1:A:1382:ARG:NH1	2.35	0.42
1:A:2384:MET:H	1:A:2384:MET:HG2	1.57	0.42
1:A:2431:ILE:HG12	1:B:2425:ARG:NH2	2.35	0.42
1:B:676:SER:O	1:B:679:LEU:HB2	2.19	0.42
1:B:686:ALA:C	1:B:688:TRP:N	2.73	0.42
1:B:1001:GLY:O	1:B:1002:LEU:C	2.62	0.42
1:B:1056:LEU:HA	1:B:1059:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:PRO:HB2	1:B:1066:PRO:HD3	2.00	0.42
1:B:1163:LYS:HA	1:B:1163:LYS:HD3	1.69	0.42
1:B:1181:ALA:HB1	1:B:1302:PHE:HD1	1.85	0.42
1:C:639:ILE:O	1:C:643:SER:OG	2.35	0.42
1:A:481:TYR:HD2	1:A:483:SER:HB3	1.85	0.42
1:A:494:CYS:CA	1:A:497:TRP:HD1	2.32	0.42
1:A:994:ASP:C	1:A:996:GLY:H	2.26	0.42
1:B:648:VAL:HA	1:B:651:THR:HG22	2.02	0.42
1:B:826:PHE:O	1:B:830:ILE:HG12	2.19	0.42
1:B:1637:LEU:HD23	1:B:1637:LEU:HA	1.77	0.42
1:C:1916:PHE:CE2	1:C:1937:TYR:HE2	2.37	0.42
1:A:1628:MET:HE3	1:A:1718:PHE:CE2	2.54	0.42
1:A:2245:PHE:HB3	1:A:2339:PHE:HE2	1.83	0.42
1:B:1349:LYS:O	1:B:1352:LYS:HB3	2.19	0.42
1:B:2344:PHE:HA	1:B:2345:PRO:HD3	1.90	0.42
1:C:1344:ASN:HA	1:C:1347:ILE:HG22	2.01	0.42
1:C:1349:LYS:O	1:C:1352:LYS:HB3	2.19	0.42
1:C:2123:ASP:OD1	1:C:2123:ASP:C	2.63	0.42
1:C:2272:ILE:HD13	1:C:2272:ILE:HA	1.80	0.42
1:A:1176:MET:CE	1:A:1179:LEU:HD22	2.36	0.42
1:A:1305:ILE:HD12	1:A:1306:ALA:N	2.34	0.42
1:B:991:PHE:CA	1:B:995:TYR:H	2.33	0.42
1:C:1163:LYS:HA	1:C:1163:LYS:HD3	1.69	0.42
1:A:517:ILE:HD12	1:A:520:LEU:HD12	2.02	0.42
1:A:687:PHE:CD2	1:A:764:HIS:NE2	2.81	0.42
1:A:875:MET:O	1:A:879:LEU:HG	2.20	0.42
1:A:991:PHE:CA	1:A:995:TYR:H	2.33	0.42
1:A:1056:LEU:HA	1:A:1059:PHE:HB2	2.01	0.42
1:A:1249:LEU:HD21	1:A:1281:LEU:CD2	2.48	0.42
1:A:1904:GLN:HE21	1:A:1951:ILE:HD12	1.85	0.42
1:C:449:SER:O	1:C:452:SER:HB3	2.20	0.42
1:C:989:ILE:O	1:C:992:LEU:HB3	2.19	0.42
1:A:1020:LEU:HD13	1:A:1024:GLN:HE22	1.84	0.42
1:A:1381:GLU:O	1:A:1381:GLU:HG2	2.18	0.42
1:A:1939:ILE:HD13	1:A:1939:ILE:HA	1.87	0.42
1:B:690:THR:C	1:B:692:THR:H	2.28	0.42
1:B:875:MET:O	1:B:879:LEU:HG	2.20	0.42
1:B:1152:ILE:HG13	1:B:1153:ASP:H	1.85	0.42
1:B:1305:ILE:HD12	1:B:1306:ALA:N	2.34	0.42
1:B:1343:LYS:HE2	1:B:1343:LYS:HB3	1.86	0.42
1:B:1686:TRP:CH2	1:B:1698:ASP:CB	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2123:ASP:OD1	1:B:2123:ASP:C	2.62	0.42
1:C:1181:ALA:HB1	1:C:1302:PHE:HD1	1.85	0.42
1:C:1904:GLN:HE21	1:C:1951:ILE:HD12	1.85	0.42
1:C:2120:ALA:HB2	1:C:2318:LYS:HG2	2.02	0.42
1:A:529:MET:O	1:A:531:ILE:N	2.49	0.41
1:A:2075:MET:HE1	1:A:2108:MET:HE1	2.02	0.41
1:B:449:SER:O	1:B:452:SER:HB3	2.20	0.41
1:B:490:LEU:C	1:B:490:LEU:CD2	2.91	0.41
1:C:1070:ILE:HD12	1:C:1070:ILE:HA	1.84	0.41
1:C:1846:MET:HE3	1:C:1846:MET:HB2	1.71	0.41
1:B:517:ILE:HD12	1:B:520:LEU:HD12	2.02	0.41
1:B:848:ALA:O	1:B:851:ILE:HD12	2.20	0.41
1:B:1148:GLN:H	1:B:1148:GLN:HG2	1.66	0.41
1:B:1378:LYS:HD2	1:B:1382:ARG:NH1	2.35	0.41
1:B:2120:ALA:HB2	1:B:2318:LYS:HG2	2.02	0.41
1:C:494:CYS:CA	1:C:497:TRP:HD1	2.32	0.41
1:C:633:LYS:HA	1:C:633:LYS:HD3	1.63	0.41
1:C:1180:ALA:HA	1:C:1183:ILE:HD12	2.01	0.41
1:C:1281:LEU:HD23	1:C:1284:LEU:HB2	2.02	0.41
1:A:853:LEU:HB2	1:A:878:TYR:HD2	1.86	0.41
1:A:2350:LYS:HG2	1:A:2353:LYS:CG	2.49	0.41
1:C:529:MET:O	1:C:531:ILE:N	2.49	0.41
1:C:648:VAL:HA	1:C:651:THR:HG22	2.02	0.41
1:C:1152:ILE:HG13	1:C:1153:ASP:H	1.85	0.41
1:C:1305:ILE:HD12	1:C:1306:ALA:N	2.34	0.41
1:C:2075:MET:HE1	1:C:2108:MET:HE1	2.02	0.41
1:A:454:GLY:O	1:A:455:MET:C	2.63	0.41
1:A:633:LYS:HD3	1:A:633:LYS:HA	1.63	0.41
1:A:848:ALA:O	1:A:851:ILE:HD12	2.20	0.41
1:A:1181:ALA:HB1	1:A:1302:PHE:HD1	1.85	0.41
1:B:2350:LYS:HG2	1:B:2353:LYS:CG	2.49	0.41
1:B:2431:ILE:HG12	1:C:2425:ARG:NH2	2.35	0.41
1:C:2106:LEU:HD11	1:C:2152:LEU:HD21	2.01	0.41
1:B:1190:ALA:HA	1:B:1193:TYR:CD1	2.53	0.41
1:B:1281:LEU:HD23	1:B:1284:LEU:HB2	2.02	0.41
1:C:517:ILE:HD12	1:C:520:LEU:HD12	2.02	0.41
1:C:853:LEU:HB2	1:C:878:TYR:HD2	1.86	0.41
1:C:1157:SER:O	1:C:1161:TYR:N	2.48	0.41
1:C:1320:TRP:CE3	1:C:1320:TRP:HA	2.56	0.41
1:A:460:THR:CG2	1:A:464:PHE:HE1	2.23	0.41
1:A:1000:PHE:HB3	1:A:1001:GLY:H	1.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:LEU:HA	1:A:1235:ILE:HG22	2.03	0.41
1:A:1610:ILE:HD12	1:A:1610:ILE:HA	1.87	0.41
1:A:2425:ARG:NH2	1:C:2431:ILE:HG12	2.35	0.41
1:B:679:LEU:HD13	1:B:679:LEU:HA	1.85	0.41
1:B:1010:GLY:O	1:B:1013:ILE:HG22	2.21	0.41
1:C:1686:TRP:CH2	1:C:1698:ASP:CB	3.02	0.41
1:A:449:SER:O	1:A:452:SER:HB3	2.20	0.41
1:A:833:ILE:HA	1:A:836:VAL:HG12	2.03	0.41
1:A:1157:SER:O	1:A:1159:VAL:N	2.54	0.41
1:A:2064:TRP:HD1	1:B:1871:PRO:HG3	1.69	0.41
1:B:565:LEU:O	1:B:568:PRO:HD2	2.21	0.41
1:B:652:CYS:O	1:B:652:CYS:SG	2.79	0.41
1:B:1232:LEU:HA	1:B:1235:ILE:HG22	2.03	0.41
1:C:690:THR:C	1:C:692:THR:H	2.28	0.41
1:C:833:ILE:HA	1:C:836:VAL:HG12	2.03	0.41
1:C:848:ALA:O	1:C:851:ILE:HD12	2.20	0.41
1:A:652:CYS:O	1:A:652:CYS:SG	2.79	0.41
1:A:1152:ILE:HG13	1:A:1153:ASP:H	1.85	0.41
1:A:1320:TRP:CE3	1:A:1320:TRP:HA	2.56	0.41
1:A:1637:LEU:HD23	1:A:1637:LEU:HA	1.77	0.41
1:B:633:LYS:HA	1:B:633:LYS:HD3	1.63	0.41
1:B:1904:GLN:HE21	1:B:1951:ILE:HD12	1.85	0.41
1:B:1916:PHE:CE2	1:B:1937:TYR:HE2	2.37	0.41
1:C:831:SER:O	1:C:834:VAL:HG22	2.21	0.41
1:C:991:PHE:CA	1:C:995:TYR:H	2.33	0.41
1:A:648:VAL:HA	1:A:651:THR:HG22	2.02	0.41
1:A:830:ILE:HD13	1:A:830:ILE:HA	1.89	0.41
1:A:831:SER:O	1:A:834:VAL:HG22	2.21	0.41
1:A:1191:LEU:O	1:A:1195:ILE:HG12	2.21	0.41
1:A:1711:LEU:HB3	1:A:1712:TRP:H	1.55	0.41
1:A:2008:ASN:OD1	1:C:2378:THR:OG1	2.33	0.41
1:A:2120:ALA:HB2	1:A:2318:LYS:HG2	2.02	0.41
1:B:502:THR:O	1:B:505:SER:OG	2.38	0.41
1:B:699:ILE:O	1:B:702:LEU:HG	2.21	0.41
1:B:836:VAL:O	1:B:840:ILE:HG13	2.21	0.41
1:B:1157:SER:O	1:B:1159:VAL:N	2.54	0.41
1:B:1330:ARG:HH11	1:B:1330:ARG:HB3	1.86	0.41
1:B:2331:ARG:HH11	1:B:2331:ARG:HD3	1.64	0.41
1:C:1016:ARG:NH2	1:C:1020:LEU:HD12	2.36	0.41
1:C:1045:PHE:HB3	1:C:1049:TYR:CZ	2.56	0.41
1:C:1176:MET:CE	1:C:1179:LEU:HD22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1191:LEU:O	1:C:1195:ILE:HG12	2.21	0.41
1:C:2197:ASP:HA	1:C:2198:PRO:HD2	1.68	0.41
1:A:502:THR:O	1:A:505:SER:OG	2.38	0.41
1:A:1010:GLY:O	1:A:1013:ILE:HG22	2.21	0.41
1:A:1623:ILE:HG13	1:A:1941:SER:OG	2.21	0.41
1:A:1664:THR:O	1:A:1667:VAL:HG12	2.21	0.41
1:A:1940:LYS:HD2	1:A:1940:LYS:HA	1.76	0.41
1:B:1013:ILE:HD12	1:B:1013:ILE:HA	1.81	0.41
1:B:1320:TRP:HA	1:B:1320:TRP:CE3	2.56	0.41
1:C:1022:ALA:O	1:C:1025:CYS:HB2	2.21	0.41
1:A:1045:PHE:HB3	1:A:1049:TYR:CZ	2.56	0.40
1:A:2208:LYS:HG2	1:A:2210:TRP:CZ2	2.56	0.40
1:C:483:SER:HA	1:C:546:ILE:HD11	2.03	0.40
1:C:652:CYS:O	1:C:652:CYS:SG	2.79	0.40
1:A:699:ILE:O	1:A:702:LEU:HG	2.21	0.40
1:A:871:PHE:O	1:A:874:PHE:HB2	2.21	0.40
1:A:1209:VAL:HA	1:A:1329:TYR:HB3	2.03	0.40
1:A:1367:ARG:O	1:A:1371:ALA:N	2.49	0.40
1:B:483:SER:C	1:B:486:GLY:N	2.74	0.40
1:B:521:LEU:H	1:B:521:LEU:HG	1.63	0.40
1:B:871:PHE:O	1:B:874:PHE:HB2	2.21	0.40
1:B:2118:ASN:CG	1:B:2144:LYS:HE3	2.47	0.40
1:C:848:ALA:HA	1:C:851:ILE:HD12	2.03	0.40
1:C:1010:GLY:O	1:C:1013:ILE:HG22	2.21	0.40
1:C:1266:ARG:O	1:C:1266:ARG:CG	2.69	0.40
1:C:1330:ARG:HB3	1:C:1330:ARG:HH11	1.86	0.40
1:C:1641:SER:HA	1:C:1656:PHE:CZ	2.49	0.40
1:C:2208:LYS:HG2	1:C:2210:TRP:CZ2	2.56	0.40
1:A:529:MET:C	1:A:531:ILE:H	2.30	0.40
1:A:848:ALA:HA	1:A:851:ILE:HD12	2.03	0.40
1:A:876:CYS:HA	1:A:879:LEU:HD11	2.04	0.40
1:A:1281:LEU:HD23	1:A:1284:LEU:HB2	2.02	0.40
1:A:1343:LYS:HE2	1:A:1343:LYS:HB3	1.86	0.40
1:B:977:HIS:HB2	1:B:980:HIS:HB2	2.03	0.40
1:B:1191:LEU:O	1:B:1195:ILE:HG12	2.21	0.40
1:B:1212:SER:HB3	1:B:1215:ARG:HB3	2.03	0.40
1:B:1623:ILE:HG13	1:B:1941:SER:OG	2.21	0.40
1:B:1973:MET:O	1:B:1977:LYS:HB2	2.21	0.40
1:C:481:TYR:HD2	1:C:483:SER:HB3	1.85	0.40
1:C:1232:LEU:HA	1:C:1235:ILE:HG22	2.03	0.40
1:C:1321:TYR:O	1:C:1322:PHE:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2118:ASN:CG	1:C:2144:LYS:HE3	2.47	0.40
1:C:2208:LYS:HG3	1:C:2209:SER:N	2.35	0.40
1:C:2331:ARG:HH11	1:C:2331:ARG:HD3	1.64	0.40
1:A:565:LEU:O	1:A:568:PRO:HD2	2.21	0.40
1:A:1021:ALA:HA	1:A:1024:GLN:NE2	2.37	0.40
1:A:1022:ALA:O	1:A:1025:CYS:HB2	2.22	0.40
1:A:1191:LEU:HB2	1:A:1672:PHE:CZ	2.57	0.40
1:A:2208:LYS:HG3	1:A:2209:SER:N	2.35	0.40
1:B:831:SER:O	1:B:834:VAL:HG22	2.21	0.40
1:B:833:ILE:HA	1:B:836:VAL:HG12	2.03	0.40
1:B:1116:LEU:HA	1:B:1116:LEU:HD23	1.86	0.40
1:B:1323:GLN:HE21	1:B:1327:VAL:HG23	1.86	0.40
1:B:1916:PHE:O	1:B:1917:LEU:HD23	2.21	0.40
1:B:2075:MET:HE1	1:B:2108:MET:HE1	2.02	0.40
1:B:2089:PRO:HA	1:B:2090:PRO:HD3	1.98	0.40
1:C:529:MET:C	1:C:531:ILE:H	2.30	0.40
1:C:679:LEU:HA	1:C:679:LEU:HD13	1.85	0.40
1:C:1013:ILE:HD12	1:C:1013:ILE:HA	1.82	0.40
1:C:1191:LEU:HB2	1:C:1672:PHE:CZ	2.57	0.40
1:C:1212:SER:HB3	1:C:1215:ARG:HB3	2.03	0.40
1:C:1249:LEU:HD21	1:C:1281:LEU:CD2	2.48	0.40
1:A:1323:GLN:HE21	1:A:1327:VAL:HG23	1.86	0.40
1:A:1693:ASP:OD1	1:A:1696:SER:HB3	2.22	0.40
1:B:454:GLY:O	1:B:455:MET:C	2.63	0.40
1:B:853:LEU:HB2	1:B:878:TYR:HD2	1.86	0.40
1:B:1016:ARG:NH2	1:B:1020:LEU:HD12	2.36	0.40
1:C:565:LEU:O	1:C:568:PRO:HD2	2.21	0.40
1:C:809:LYS:HB3	1:C:809:LYS:HE3	1.73	0.40
1:C:1021:ALA:HA	1:C:1024:GLN:NE2	2.37	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	1918/2442 (78%)	1711 (89%)	171 (9%)	36 (2%)	6	33
1	B	1918/2442 (78%)	1711 (89%)	171 (9%)	36 (2%)	6	33
1	C	1918/2442 (78%)	1712 (89%)	170 (9%)	36 (2%)	6	33
All	All	5754/7326 (78%)	5134 (89%)	512 (9%)	108 (2%)	8	33

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ILE
1	A	289	TRP
1	A	482	HIS
1	A	691	LEU
1	A	983	ARG
1	A	989	ILE
1	A	997	PHE
1	A	1079	PRO
1	A	1158	TYR
1	A	1247	VAL
1	A	1253	ASP
1	A	1271	ILE
1	A	1831	LEU
1	B	259	ILE
1	B	289	TRP
1	B	482	HIS
1	B	691	LEU
1	B	983	ARG
1	B	989	ILE
1	B	997	PHE
1	B	1079	PRO
1	B	1158	TYR
1	B	1247	VAL
1	B	1253	ASP
1	B	1271	ILE
1	B	1831	LEU
1	C	259	ILE
1	C	289	TRP
1	C	482	HIS
1	C	691	LEU
1	C	983	ARG
1	C	989	ILE
1	C	997	PHE
1	C	1079	PRO

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Mol	Chain	Res	Type
1	C	1158	TYR
1	C	1247	VAL
1	C	1253	ASP
1	C	1271	ILE
1	C	1831	LEU
1	A	106	ILE
1	A	116	THR
1	A	496	LEU
1	A	985	LEU
1	A	990	GLN
1	A	1000	PHE
1	A	1333	VAL
1	A	1335	LEU
1	A	1379	GLN
1	A	1715	VAL
1	A	1872	VAL
1	A	2347	PHE
1	A	2352	PHE
1	B	106	ILE
1	B	116	THR
1	B	496	LEU
1	B	985	LEU
1	B	990	GLN
1	B	1000	PHE
1	B	1333	VAL
1	B	1335	LEU
1	B	1379	GLN
1	B	1715	VAL
1	B	1872	VAL
1	B	2347	PHE
1	B	2352	PHE
1	C	106	ILE
1	C	116	THR
1	C	496	LEU
1	C	985	LEU
1	C	990	GLN
1	C	1000	PHE
1	C	1333	VAL
1	C	1335	LEU
1	C	1379	GLN
1	C	1715	VAL
1	C	1872	VAL

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Mol	Chain	Res	Type
1	C	2347	PHE
1	C	2352	PHE
1	A	527	LEU
1	A	978	HIS
1	A	1157	SER
1	B	527	LEU
1	B	978	HIS
1	B	1157	SER
1	C	527	LEU
1	C	978	HIS
1	C	1157	SER
1	A	1249	LEU
1	A	1388	ASP
1	A	2272	ILE
1	A	2345	PRO
1	B	1249	LEU
1	B	1388	ASP
1	B	2272	ILE
1	B	2345	PRO
1	C	1249	LEU
1	C	1388	ASP
1	C	2272	ILE
1	C	2345	PRO
1	A	984	SER
1	A	1339	GLY
1	B	984	SER
1	B	1339	GLY
1	C	984	SER
1	C	1339	GLY
1	A	1066	PRO
1	B	1066	PRO
1	C	1066	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1449/2141 (68%)	1417 (98%)	32 (2%)	45	65
1	B	1449/2141 (68%)	1418 (98%)	31 (2%)	47	66
1	C	1449/2141 (68%)	1416 (98%)	33 (2%)	44	64
All	All	4347/6423 (68%)	4251 (98%)	96 (2%)	45	65

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	TYR
1	A	521	LEU
1	A	525	TYR
1	A	529	MET
1	A	559	LEU
1	A	949	SER
1	A	1056	LEU
1	A	1078	ILE
1	A	1096	SER
1	A	1115	LEU
1	A	1168	HIS
1	A	1196	PHE
1	A	1249	LEU
1	A	1264	ILE
1	A	1266	ARG
1	A	1267	GLN
1	A	1284	LEU
1	A	1294	GLU
1	A	1296	LYS
1	A	1355	ASN
1	A	1377	GLN
1	A	1386	GLU
1	A	1665	GLU
1	A	1698	ASP
1	A	1894	ARG
1	A	2035	ILE
1	A	2041	VAL
1	A	2042	LYS
1	A	2073	ILE
1	A	2331	ARG
1	A	2366	VAL
1	A	2433	TRP
1	B	467	TYR
1	B	521	LEU

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Mol	Chain	Res	Type
1	B	525	TYR
1	B	529	MET
1	B	559	LEU
1	B	949	SER
1	B	1056	LEU
1	B	1078	ILE
1	B	1096	SER
1	B	1115	LEU
1	B	1168	HIS
1	B	1196	PHE
1	B	1249	LEU
1	B	1264	ILE
1	B	1266	ARG
1	B	1267	GLN
1	B	1284	LEU
1	B	1294	GLU
1	B	1296	LYS
1	B	1355	ASN
1	B	1377	GLN
1	B	1386	GLU
1	B	1665	GLU
1	B	1698	ASP
1	B	1894	ARG
1	B	2035	ILE
1	B	2041	VAL
1	B	2042	LYS
1	B	2331	ARG
1	B	2366	VAL
1	B	2433	TRP
1	C	467	TYR
1	C	521	LEU
1	C	525	TYR
1	C	529	MET
1	C	559	LEU
1	C	941	SER
1	C	949	SER
1	C	1056	LEU
1	C	1078	ILE
1	C	1096	SER
1	C	1115	LEU
1	C	1168	HIS
1	C	1196	PHE

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Mol	Chain	Res	Type
1	C	1249	LEU
1	C	1264	ILE
1	C	1266	ARG
1	C	1267	GLN
1	C	1284	LEU
1	C	1294	GLU
1	C	1296	LYS
1	C	1355	ASN
1	C	1377	GLN
1	C	1386	GLU
1	C	1665	GLU
1	C	1698	ASP
1	C	1894	ARG
1	C	2035	ILE
1	C	2041	VAL
1	C	2042	LYS
1	C	2073	ILE
1	C	2331	ARG
1	C	2366	VAL
1	C	2433	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2201	ASN
1	B	717	ASN
1	B	1953	ASN
1	B	2201	ASN
1	C	717	ASN
1	C	1931	HIS
1	C	2201	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

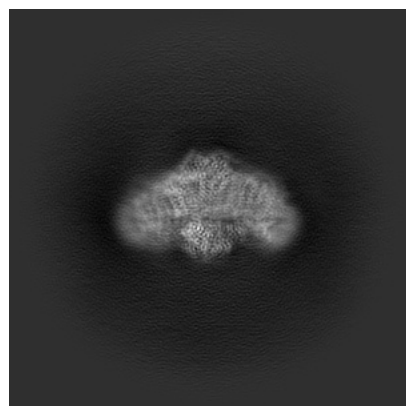
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74281. These allow visual inspection of the internal detail of the map and identification of artifacts.

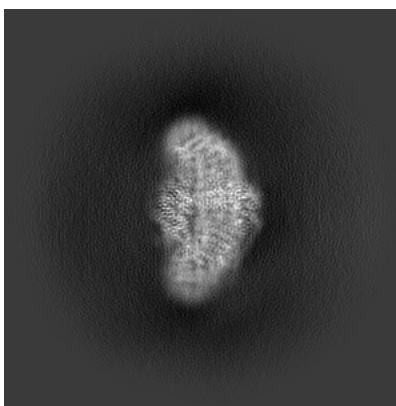
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

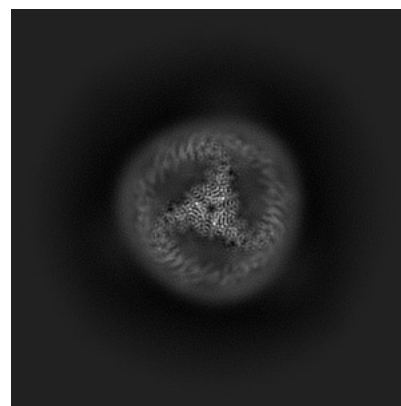
6.1.1 Primary map



X

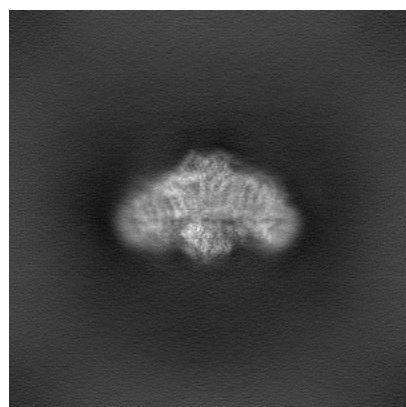


Y

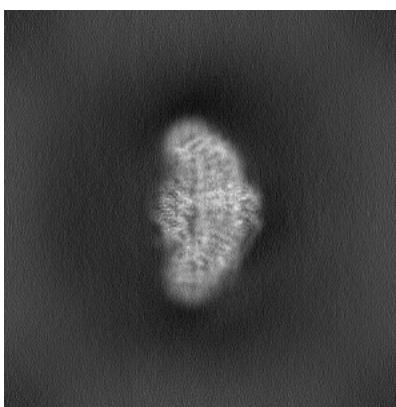


Z

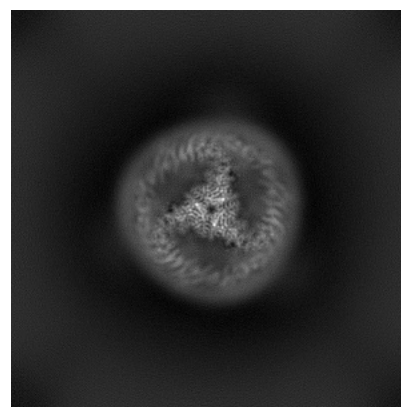
6.1.2 Raw map



X



Y

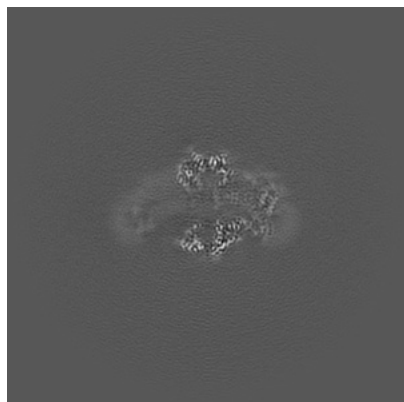


Z

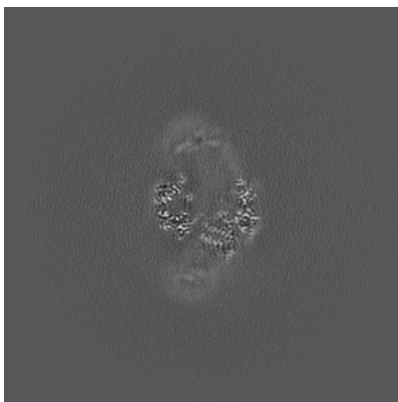
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

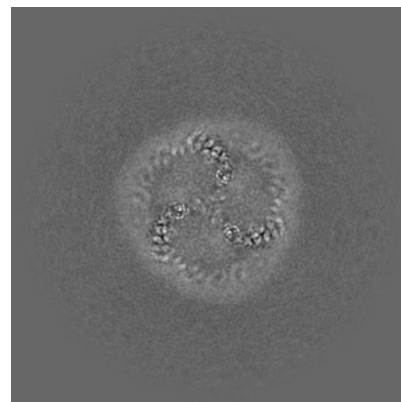
6.2.1 Primary map



X Index: 224

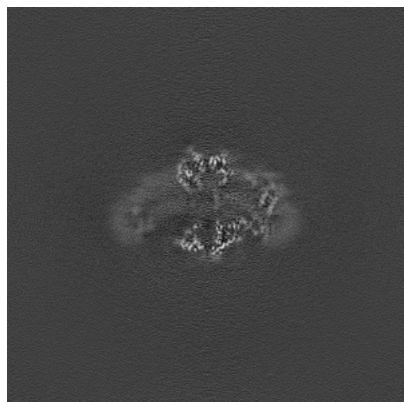


Y Index: 224

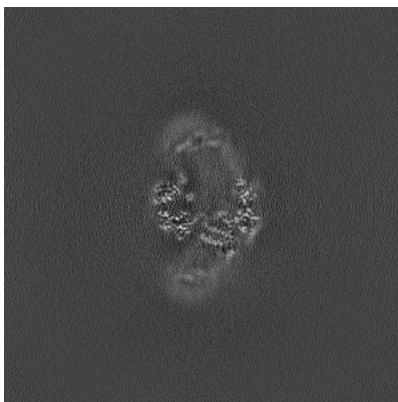


Z Index: 224

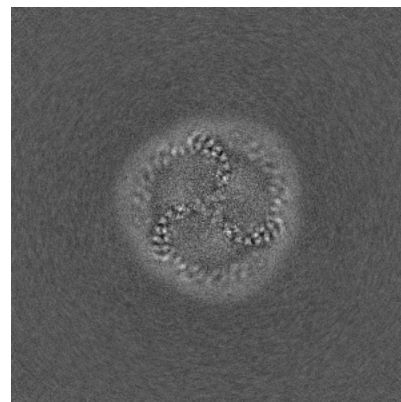
6.2.2 Raw map



X Index: 224



Y Index: 224

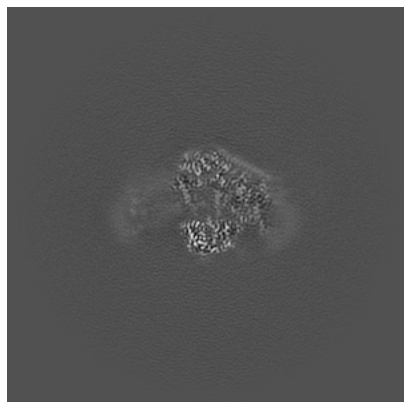


Z Index: 224

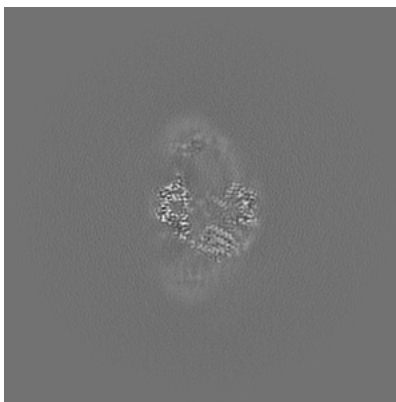
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

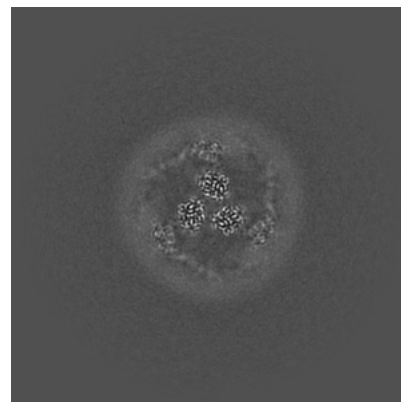
6.3.1 Primary map



X Index: 236

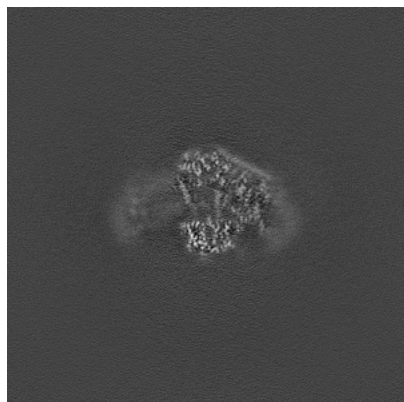


Y Index: 216

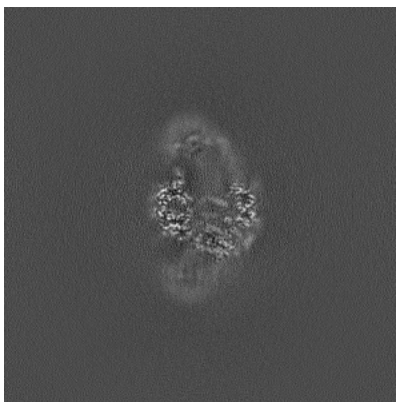


Z Index: 197

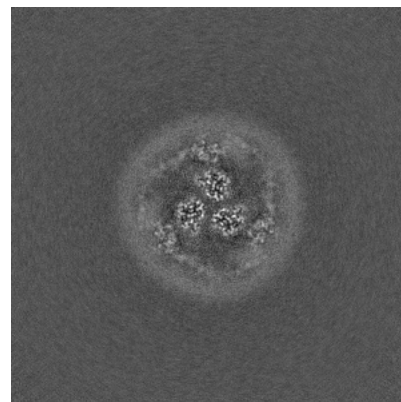
6.3.2 Raw map



X Index: 236



Y Index: 218

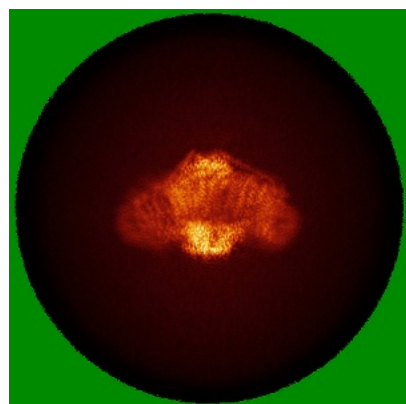


Z Index: 198

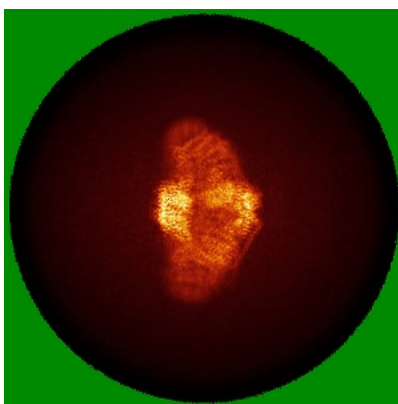
The images above show the largest variance slices of the map in three orthogonal directions.

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

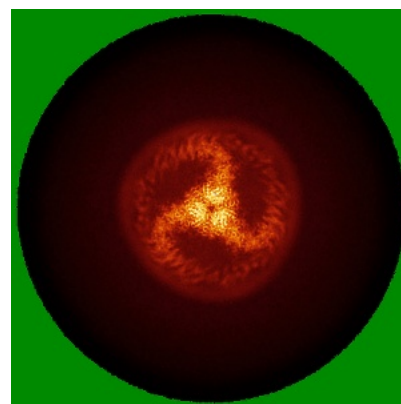
6.4.1 Primary map



X

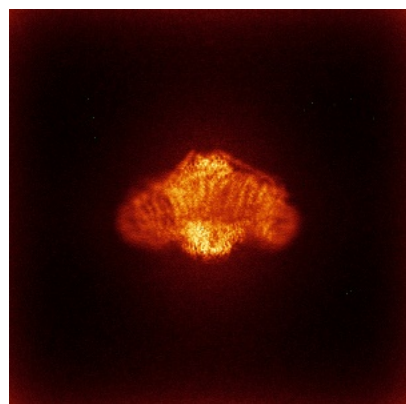


Y

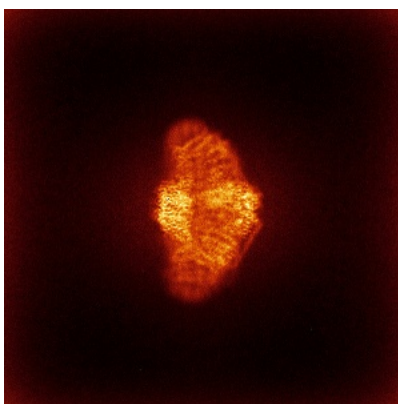


Z

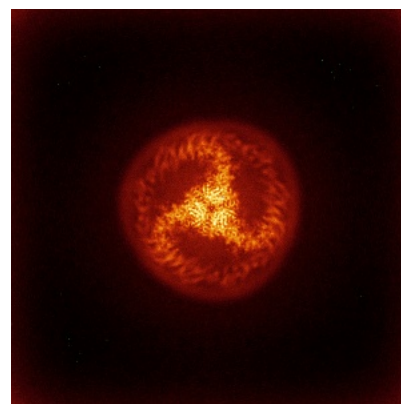
6.4.2 Raw map



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 0.0561. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

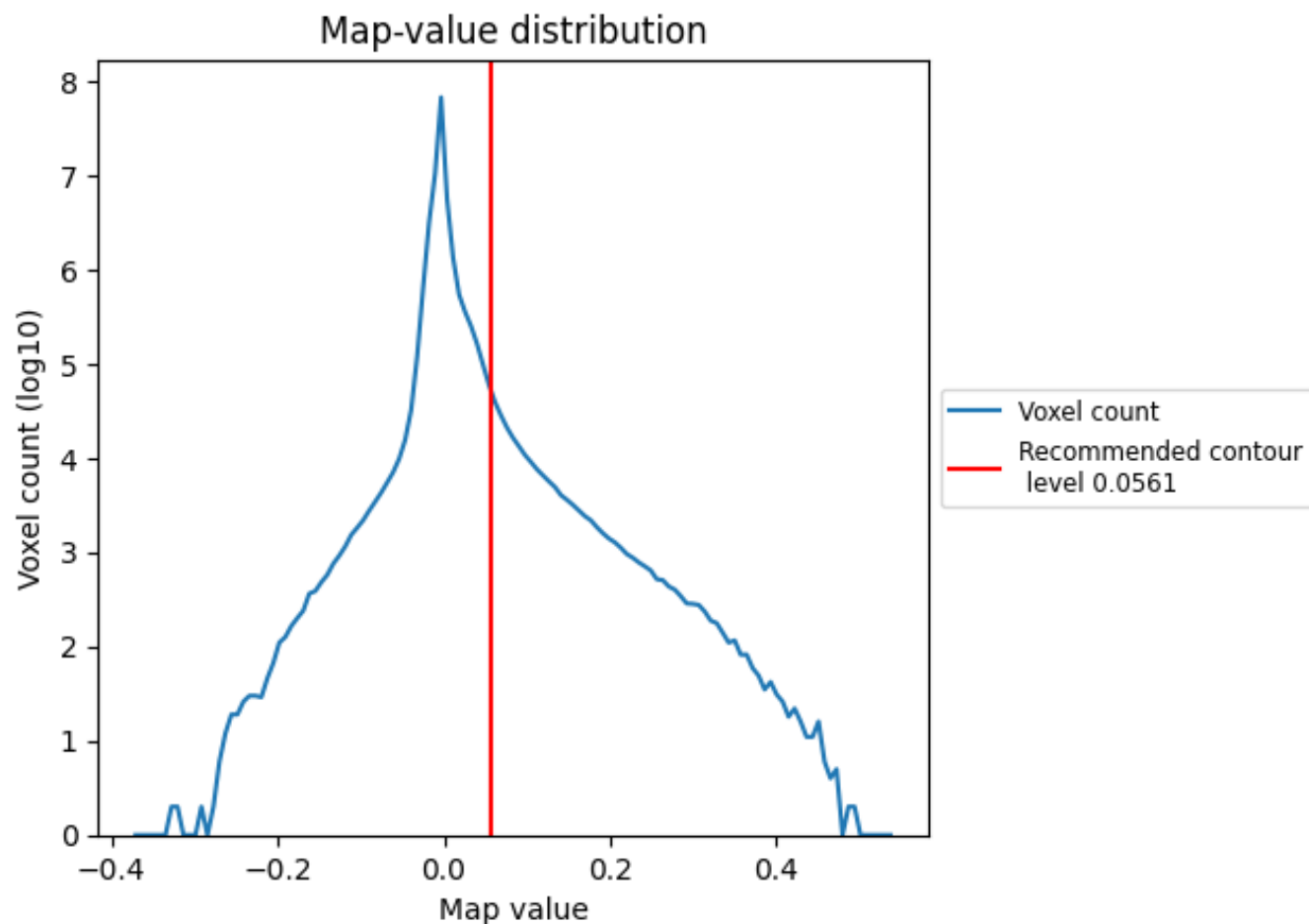
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

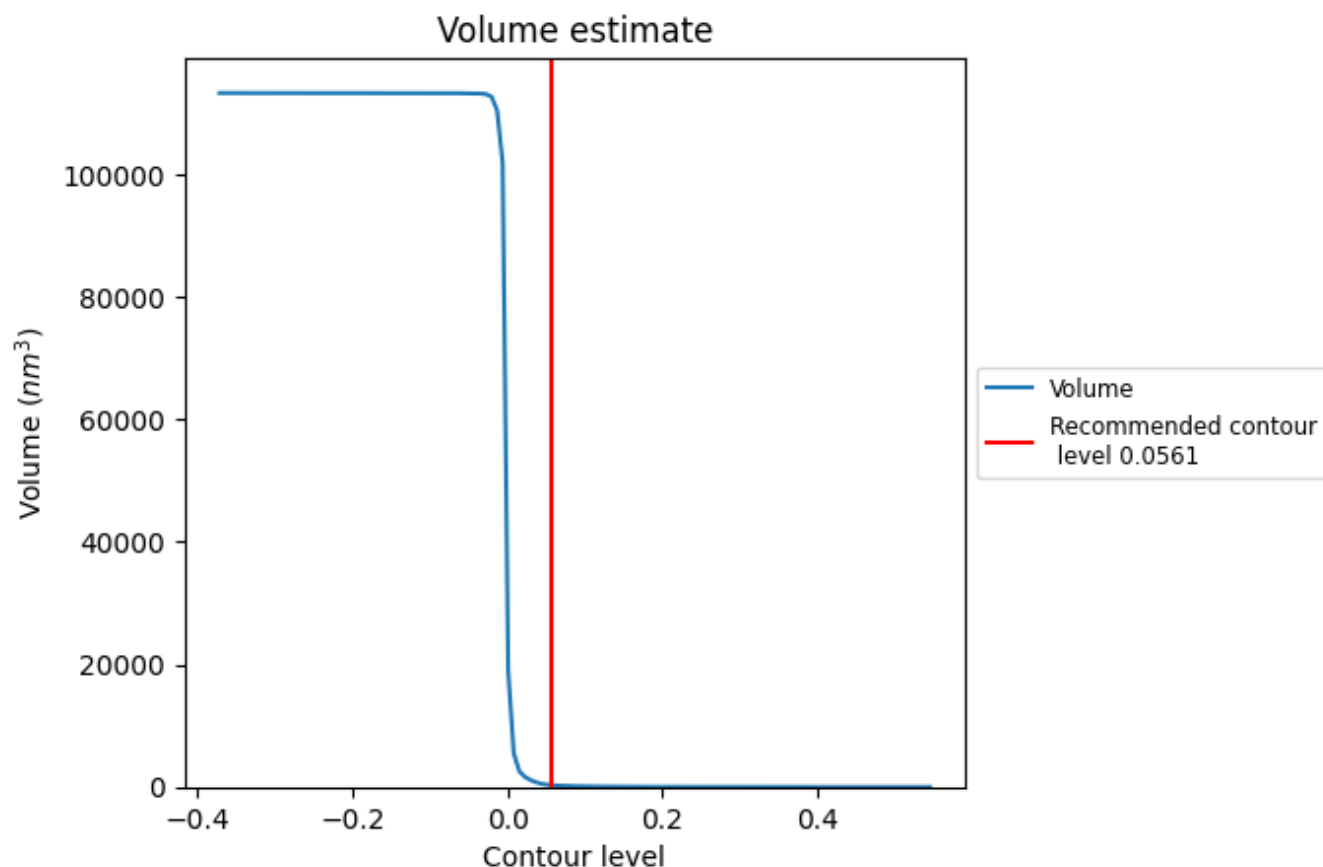
This section contains the results of statistical analysis of the map.

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.

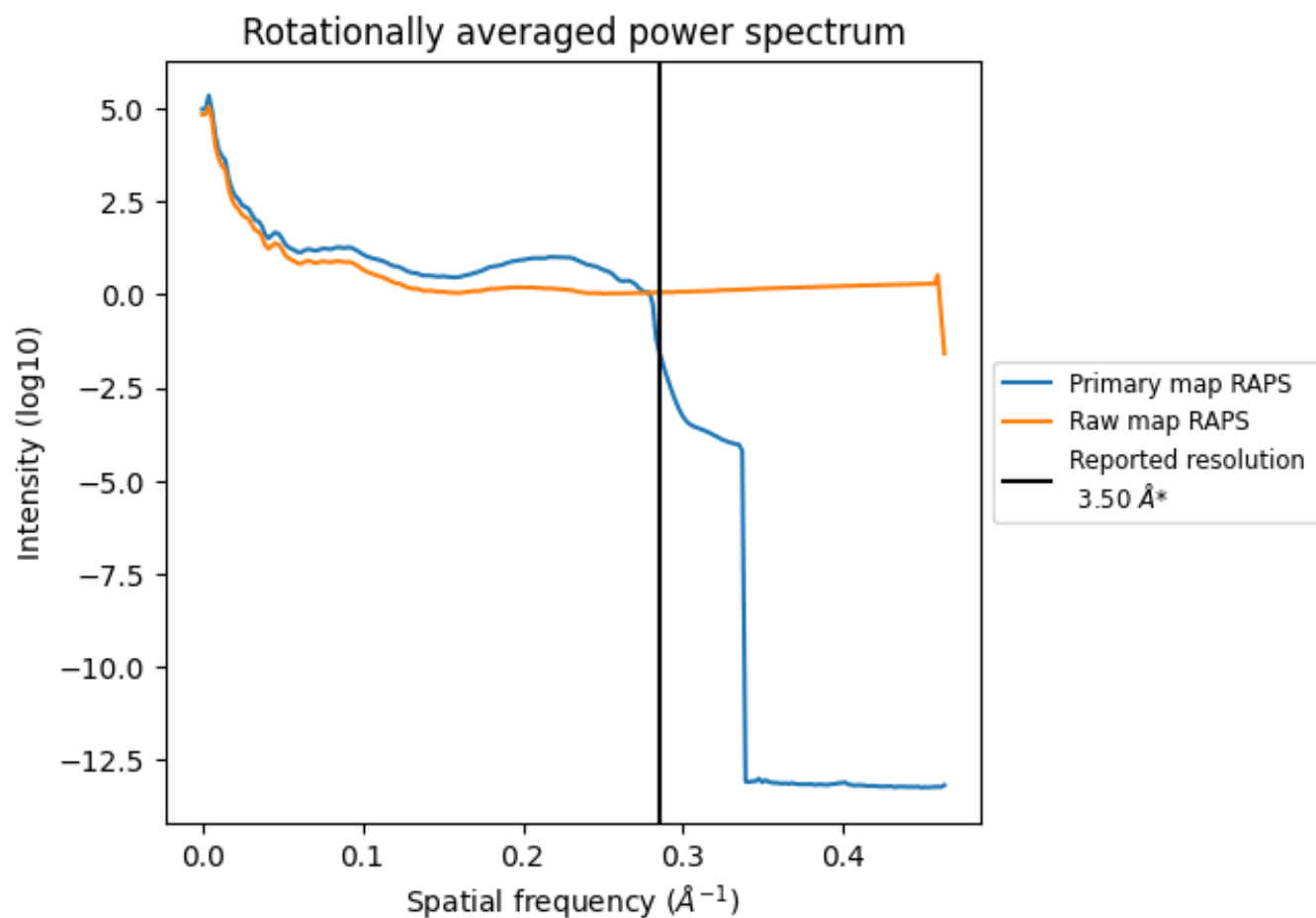
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 305 nm^3 ; this corresponds to an approximate mass of 276 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

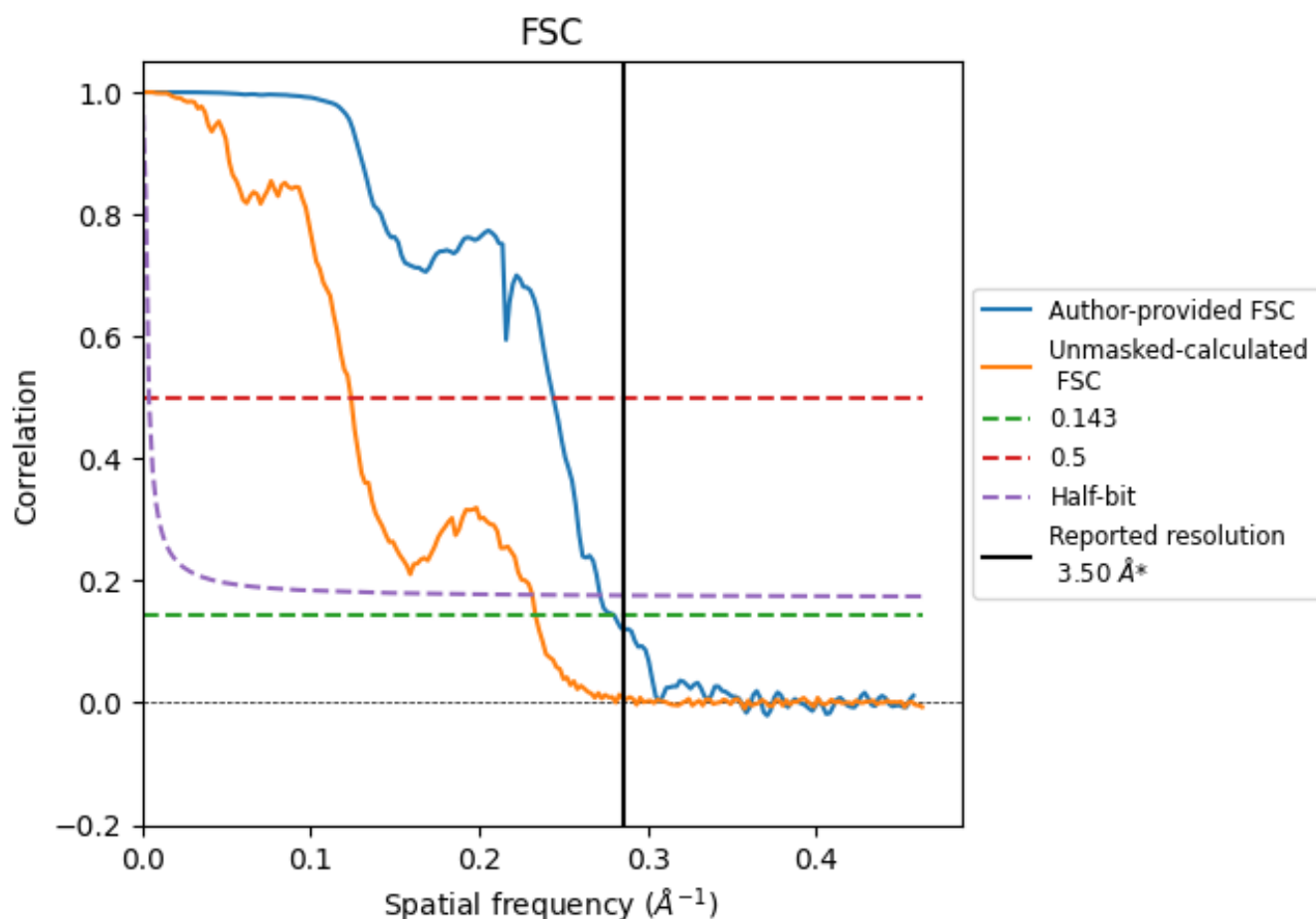


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

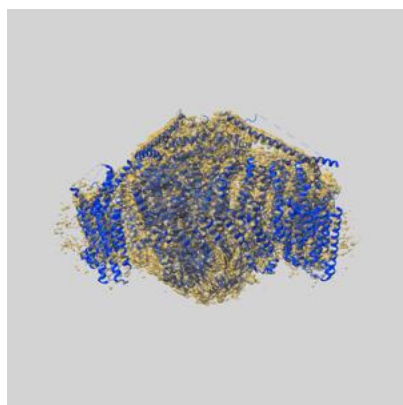
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.57	4.10	3.68
Unmasked-calculated*	4.28	8.06	4.32

*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 4.28 differs from the reported value 3.5 by more than 10 %

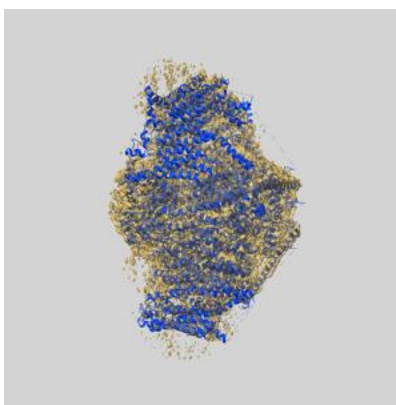
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74281 and PDB model 9ZIS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

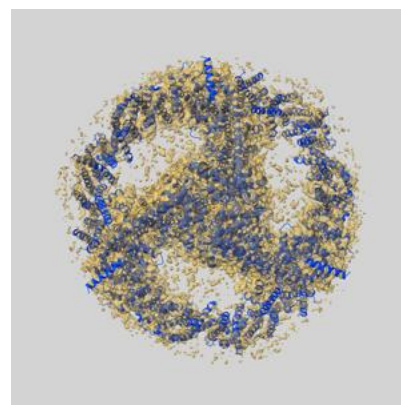
9.1 Map-model overlay [i](#)



X



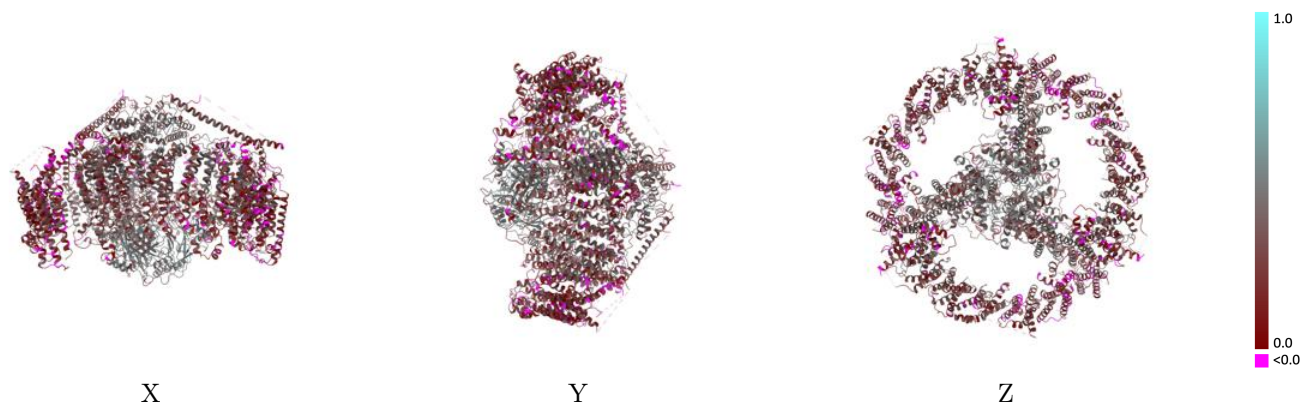
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0561 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

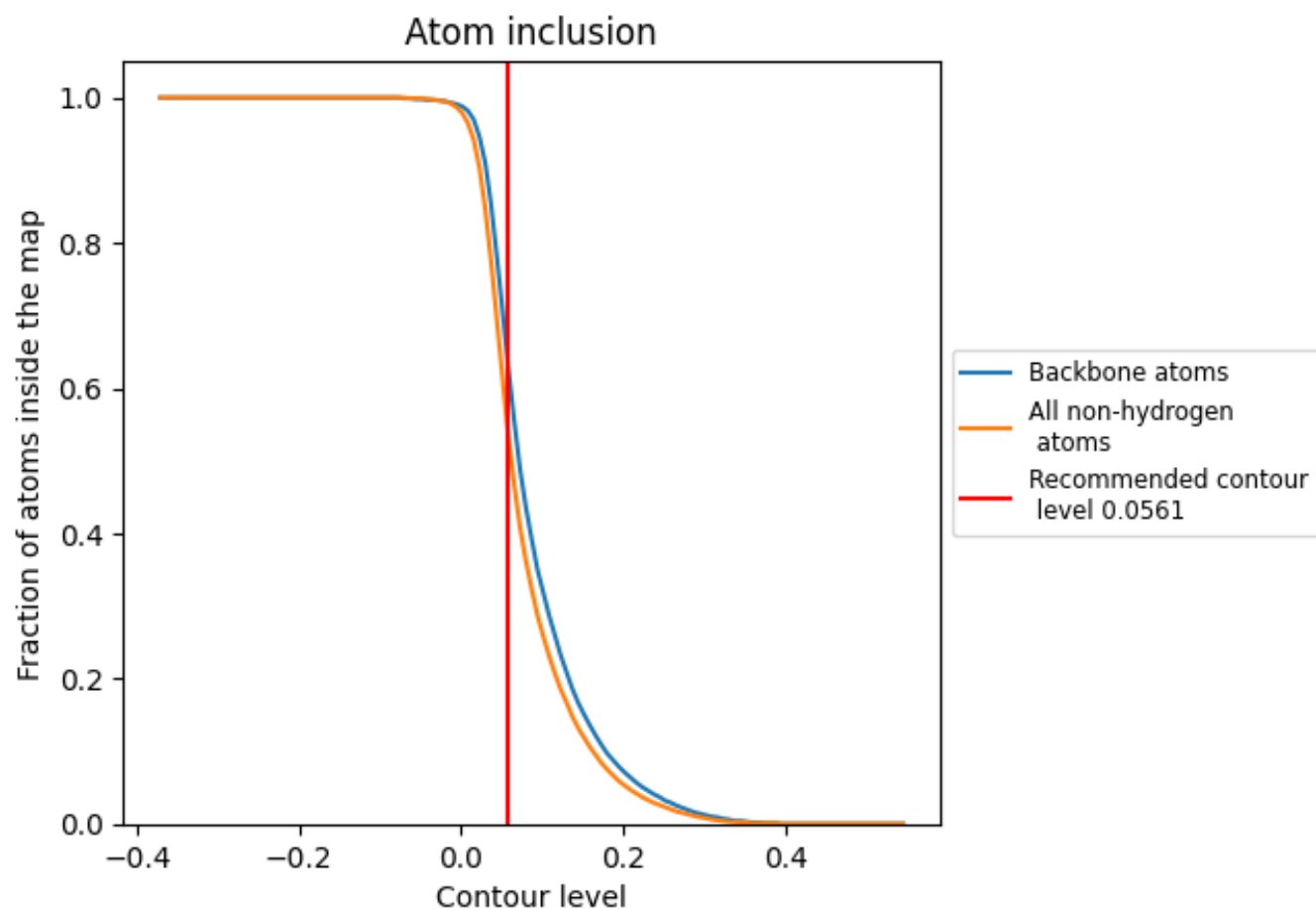


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 55% 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 (0.0561) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5540	0.3000
A	0.5540	0.2990
B	0.5530	0.3010
C	0.5540	0.3000

