



## Full wwPDB EM Validation Report ⓘ

Aug 25, 2025 – 10:15 AM JST

PDB ID : 9J9F / pdb\_00009j9f  
EMDB ID : EMD-61270  
Title : Bovine ABCC1 conformation 1  
Authors : Zhong, C.; Wang, F.; Liu, Z.; Yu, G.  
Deposited on : 2024-08-22  
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

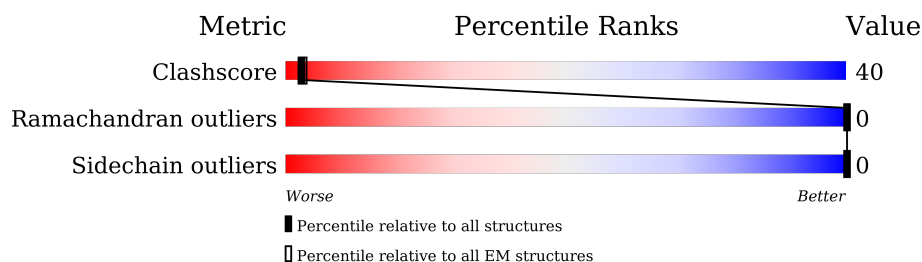
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1530	<div> <div>20%</div> <div>46%</div> <div>45%</div> <div>8%</div> </div>

## 2 Entry composition [i](#)

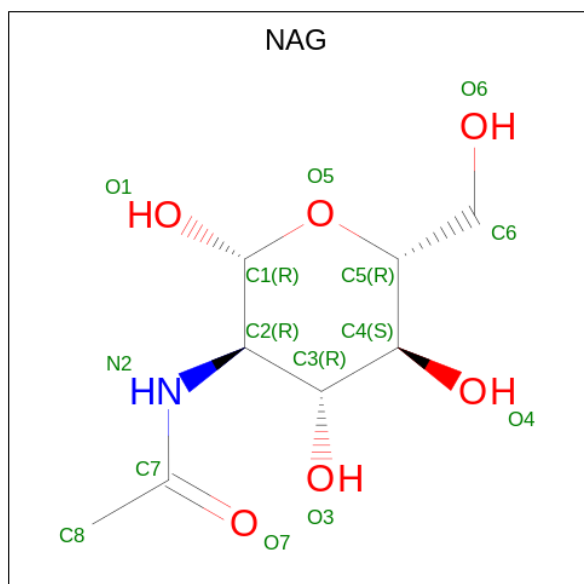
There are 2 unique types of molecules in this entry. The entry contains 10487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1400	10473	6779	1759	1883	52	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

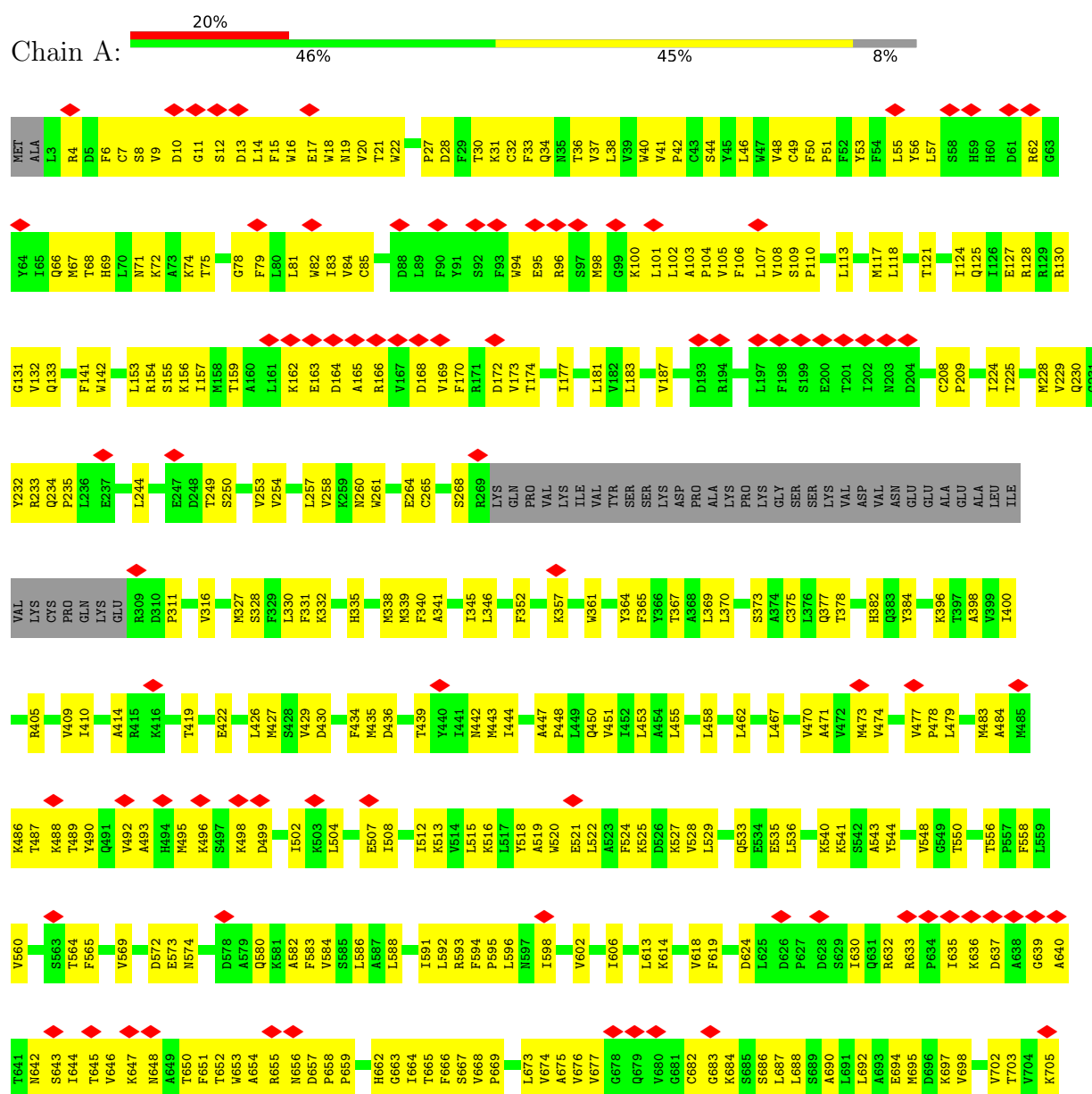


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Multidrug resistance-associated protein 1



T1489	T1490	M1491	D1492	Y1493	T1494	R1495	V1496	I1497	I1498	L1499	D1500	K1501	G1502	E1503	I1504	I1505	E1506	W1507	G1508	S1509	P1510	D1511	D1512	L1513	L1514	Q1515	Q1516	R1517	G1518	Y1521	S1522	M1523	A1524	K1525	D1526	SER	GLY	LEU	VAL																				
L1418	N1419	H1420	C1421	C1422	A1423	E1424	G1425	G1426	E1427	K1368	L1369	T1370	I1371	I1372	P1373	Q1374	D1375	P1376	V1377	L1378	F1379	S1380	G1381	S1382	L1383	R1384	M1385	L1386	L1387	D1388	P1389	F1390	S1391	Q1392	Y1393	S1394	D1395	E1396	E1397	V1398	W1399	T1400	S1401	L1402	E1403	L1404	A1405	H1406	L1407	K1408	G1409	F1410	V1411	T1412	I1413	A1414	H1415	R1416	N1417
A1358	K1359	I1360	G1361	L1362	H1363	D1364	L1365	R1366	F1367	K1368	L1369	T1370	I1371	I1372	P1373	Q1374	D1375	P1376	V1377	L1378	F1379	S1380	G1381	S1382	L1383	R1384	M1385	L1386	L1387	D1388	P1389	F1390	S1391	Q1392	Y1393	S1394	D1395	E1396	E1397	V1398	W1399	T1400	S1401	L1402	E1403	L1404	A1405	H1406	L1407	K1408	G1409	F1410	V1411	T1412	I1413	A1414	H1415	R1416	N1417
Y1297	G1298	L1299	R1300	Y1301	R1302	E1303	D1304	L1305	D1306	L1307	V1308	L1309	K1310	H1311	I1312	M1313	V1314	T1315	I1316	D1317	G1318	G1319	E1320	K1321	V1322	G1323	G1326	R1327	T1328	G1329	A1330	G1331	K1332	S1333	S1334	L1335	T1336	L1337	G1338	L1339	R1340	I1341	I1342	K1343	E1344	S1345	A1346	E1347	G1348	E1349	T1350	I1351	I1352	D1353	D1354	I1355	N1356	I1357	
G1230	L1231	V1232	V1233	V1234	Y1235	S1236	L1237	Q1238	V1239	T1240	T1241	Y1242	W1245	L1246	V1247	R1248	M1249	M1253	E1254	T1255	W1256	I1257	V1258	A1259	R1262	L1263	E1268	T1269	E1270	K1271	E1272	A1273	P1274	W1275	Q1276	I1277	Q1278	D1279	W1280	A1281	P1282	F1283	K1284	D1285	W1286	P1287	Q1288	V1289	G1290	R1291	V1292	E1293	F1294	R1295	D1296				
S1146	R1147	S1148	P1149	Y1150	Y1151	E1156	Y1163	I1164	R1165	A1166	E1169	Q1170	E1171	R1172	F1173	I1174	R1175	Q1176	S1177	D1178	V1181	D1182	E1183	N1184	Q1185	Y1188	V1189	P1190	A1194	W1197	L1198	A1199	L1202	E1203	C1204	V1205	G1208	L1211	F1212	L1215	F1216	F1217	Q1129	R1130	F1131	Y1132	V1133	R1137	V1145										
P1059	I1060	S1061	F1062	F1063	E1064	R1065	T1066	P1067	S1068	G1069	N1070	L1071	V1072	N1073	F1074	F1075	S1076	K1077	E1078	L1079	D1083	Q1088	M1092	N1099	A1103	C1104	L1108	T1111	P1112	T1117	I1118	P1119	P1120	L1121	G1122	L1123	Y1125	F1126	F1127	V1128	Q1129	R1130	F1131	Y1132	V1133	R1137	V1145												
V957	K958	S959	S960	V961	Y962	Y965	I969	L976	F981	L982	C983	V986	V990	S991	N992	Y993	W994	L995	T999	N1005	G1006	T1007	V1013	R1014	L1015	S1016	L1021	G1022	G1026	I1027	T1028	V1029	Y1032	S1033	M1034	S1037	I1038	G1039	G1040	I1041	S1044	H1048	L1056																
M835	D836	I839	V840	M841	S842	G843	G844	K845	L846	S847	E848	G850	M854	S851	Y852	Q853	E854	F855	R857	T858	Y869	A870	S871	ALA	GLU	GLN	PRO	GLY	GLN	GLN	GLY	GLY	PRO	GLU	ASP	GLY	LEU	VAL	ALA	GLY	ASP	VAL	LYS	GLN	THR	GLY	GLN												
G770	G771	Q772	K773	V774	R775	V776	S777	L778	A779	R780	A781	V782	D785	V788	Y789	L790	L791	D792	D793	P794	L795	S796	Y797	V798	D799	A800	H801	V802	G803	K804	H805	I806	F807	E808	N809	GLN	V810	I811	G812	L816	L817	K818	N819	K820	T821	R822	L823	L824	V825	A828	I829	Y831	L832	P833	Q834				
V708	A709	Y710	V711	P712	W716	I717	Q718	N719	I720	S721	L722	R723	E724	N725	I726	L727	F728	Q731	L732	Q733	E734	R735	Y736	F737	K738	A739	V740	V741	E742	A743	C744	A745	L746	L747	P748	D749	V810	L750	E751	I752	L753	P754	S755	G756	D757	R758	I759	E760	I761	G762	E763	K764	S830	G765	V766	N767	L768	S769	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.773	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/10705	0.39	0/14593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10473	0	10103	817	0
2	A	14	0	13	2	0
All	All	10487	0	10116	817	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 40.

All (817) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:SER:O	1:A:384:TYR:CE1	1.91	1.24
1:A:1297:TYR:HA	1:A:1348:GLY:HA3	1.19	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:VAL:HB	1:A:1316:ILE:HB	1.24	1.17
1:A:742:GLU:HA	1:A:747:LEU:HD11	1.32	1.09
1:A:328:SER:C	1:A:384:TYR:HE1	1.62	1.07
1:A:1298:GLY:HA2	1:A:1309:LEU:HB2	1.31	1.06
1:A:410:ILE:HG23	1:A:414:ALA:HB3	1.36	1.05
1:A:384:TYR:OH	1:A:442:ASN:ND2	1.91	1.03
1:A:1449:ILE:HG22	1:A:1479:THR:HB	1.41	1.01
1:A:668:VAL:HG12	1:A:674:VAL:HG21	1.42	0.99
1:A:328:SER:C	1:A:384:TYR:CE1	2.37	0.98
1:A:328:SER:O	1:A:384:TYR:CD1	2.16	0.98
1:A:558:PHE:CZ	1:A:1022:GLY:HA3	1.99	0.98
1:A:636:LYS:HE3	1:A:636:LYS:HA	1.47	0.97
1:A:384:TYR:OH	1:A:442:ASN:CG	2.07	0.97
1:A:965:TYR:CE2	1:A:969:ILE:HD11	2.00	0.97
1:A:778:LEU:O	1:A:782:VAL:HG23	1.65	0.96
1:A:1276:GLN:HE22	1:A:1363:HIS:HB2	1.28	0.96
1:A:1282:PRO:HG3	1:A:1364:ASP:HB3	1.46	0.96
1:A:646:VAL:HG12	1:A:702:VAL:HG23	1.45	0.96
1:A:352:PHE:CE2	1:A:1221:ARG:HD3	2.02	0.94
1:A:507:GLU:OE2	1:A:1379:PHE:HA	1.67	0.94
1:A:162:LYS:HE3	1:A:162:LYS:HA	1.50	0.93
1:A:744:CYS:SG	1:A:746:LEU:HG	2.09	0.92
1:A:1433:GLN:O	1:A:1437:VAL:HG23	1.69	0.92
1:A:719:ASN:HD21	1:A:764:LYS:HA	1.36	0.91
1:A:1382:SER:HA	1:A:1421:GLU:HA	1.51	0.90
1:A:409:VAL:HG12	1:A:624:ASP:HB3	1.52	0.89
1:A:841:MET:HA	1:A:847:SER:H	1.37	0.89
1:A:1401:SER:O	1:A:1405:ALA:N	2.06	0.89
1:A:630:ILE:HG23	1:A:702:VAL:HG13	1.55	0.88
1:A:804:LYS:O	1:A:808:GLU:HG2	1.74	0.88
1:A:467:LEU:HA	1:A:470:VAL:HG12	1.58	0.86
1:A:1390:PHE:HB3	1:A:1392:GLN:HG2	1.55	0.85
1:A:1471:ILE:O	1:A:1476:ASP:N	2.10	0.85
1:A:462:LEU:HD21	1:A:564:THR:HG22	1.56	0.85
1:A:1470:THR:O	1:A:1475:PHE:N	2.10	0.85
1:A:444:ILE:HD11	1:A:606:ILE:CD1	2.07	0.84
1:A:499:ASP:O	1:A:502:ILE:HG22	1.76	0.84
1:A:651:PHE:HE1	1:A:697:LYS:HG3	1.42	0.84
1:A:1454:GLU:N	1:A:1483:ILE:O	2.09	0.84
1:A:328:SER:HB2	1:A:384:TYR:CE1	2.13	0.83
1:A:742:GLU:HA	1:A:747:LEU:CD1	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:HG3	1:A:316:VAL:HG22	1.59	0.83
1:A:520:TRP:CE2	1:A:1389:PRO:HG3	2.13	0.83
1:A:676:VAL:HG13	1:A:825:VAL:HG23	1.60	0.83
1:A:722:LEU:HD11	1:A:776:VAL:HG21	1.59	0.83
1:A:34:GLN:OE1	1:A:155:SER:OG	1.97	0.83
1:A:68:THR:O	1:A:72:LYS:HE2	1.78	0.82
1:A:410:ILE:CG2	1:A:414:ALA:HB3	2.09	0.82
1:A:565:PHE:O	1:A:569:VAL:HG22	1.80	0.81
1:A:646:VAL:HG23	1:A:665:THR:HA	1.61	0.81
1:A:1297:TYR:HA	1:A:1348:GLY:CA	2.07	0.81
1:A:1298:GLY:N	1:A:1347:GLU:O	2.13	0.81
1:A:27:PRO:O	1:A:154:ARG:NH2	2.13	0.81
1:A:1092:MET:HE2	1:A:1249:MET:HE3	1.60	0.81
1:A:810:VAL:HG23	1:A:811:ILE:HG13	1.60	0.81
1:A:1068:SER:O	1:A:1072:VAL:HG23	1.81	0.81
1:A:382:HIS:NE2	1:A:1199:ALA:HB1	1.96	0.80
1:A:1299:LEU:HA	1:A:1346:ALA:HB3	1.60	0.80
1:A:995:LEU:O	1:A:999:THR:HG23	1.80	0.80
1:A:1297:TYR:CA	1:A:1348:GLY:HA3	2.07	0.80
1:A:686:SER:HB3	1:A:695:MET:HE1	1.64	0.80
1:A:688:LEU:HD12	1:A:792:ASP:HB2	1.64	0.80
1:A:1070:ASN:O	1:A:1074:ARG:CD	2.31	0.79
1:A:1343:LYS:HD3	1:A:1344:GLU:N	1.96	0.79
1:A:992:ASN:ND2	1:A:1235:TYR:OH	2.15	0.79
1:A:1471:ILE:HA	1:A:1475:PHE:CB	2.12	0.79
1:A:992:ASN:HB3	1:A:1231:LEU:HD11	1.65	0.79
1:A:1495:ARG:HH21	1:A:1507:TRP:HB2	1.46	0.78
1:A:462:LEU:HD21	1:A:564:THR:CG2	2.14	0.78
1:A:1217:ALA:HB1	1:A:1229:VAL:HG22	1.66	0.78
1:A:657:ASP:HB3	1:A:658:PRO:HD2	1.65	0.77
1:A:722:LEU:HD11	1:A:776:VAL:CG2	2.14	0.77
1:A:651:PHE:CE1	1:A:697:LYS:HG3	2.20	0.77
1:A:682:CYS:O	1:A:844:GLY:N	2.17	0.76
1:A:444:ILE:HD11	1:A:606:ILE:HD11	1.64	0.76
1:A:1059:PRO:HA	1:A:1272:GLU:OE2	1.85	0.76
1:A:37:VAL:O	1:A:41:VAL:HG23	1.85	0.76
1:A:750:LEU:HA	1:A:753:LEU:HG	1.67	0.76
1:A:723:ARG:O	1:A:727:LEU:HG	1.86	0.76
1:A:1060:ILE:HG13	1:A:1342:ILE:HG23	1.67	0.76
1:A:556:THR:O	1:A:560:VAL:HG23	1.87	0.75
1:A:384:TYR:OH	1:A:442:ASN:CB	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:MET:HG2	1:A:846:ILE:HA	1.69	0.75
1:A:400:ILE:HG23	1:A:427:MET:HE2	1.69	0.75
1:A:633:ARG:HH22	1:A:639:GLY:HA3	1.51	0.74
1:A:1029:VAL:HA	1:A:1032:TYR:CE1	2.22	0.74
1:A:1294:PHE:N	1:A:1314:VAL:O	2.19	0.74
1:A:1298:GLY:O	1:A:1347:GLU:N	2.21	0.74
1:A:14:LEU:HD13	1:A:17:GLU:OE1	1.88	0.74
1:A:8:SER:HB2	1:A:13:ASP:OD1	1.87	0.74
1:A:68:THR:HG22	1:A:71:ASN:ND2	2.03	0.74
1:A:498:LYS:HB3	1:A:535:GLU:OE2	1.87	0.73
1:A:643:SER:OG	1:A:821:THR:HG21	1.88	0.73
1:A:1316:ILE:HG23	1:A:1320:GLU:OE1	1.89	0.73
1:A:686:SER:CB	1:A:695:MET:HE1	2.19	0.73
1:A:1029:VAL:HA	1:A:1032:TYR:CD1	2.24	0.73
1:A:265:CYS:O	1:A:268:SER:OG	2.06	0.73
1:A:1357:ILE:O	1:A:1360:ILE:HG22	1.89	0.73
1:A:802:VAL:O	1:A:806:ILE:HG12	1.88	0.72
1:A:1070:ASN:O	1:A:1074:ARG:HD2	1.89	0.72
1:A:846:ILE:HD11	1:A:849:MET:SD	2.29	0.72
1:A:444:ILE:HD11	1:A:602:VAL:HG12	1.70	0.72
1:A:794:PRO:HG2	1:A:795:LEU:HD12	1.72	0.72
1:A:427:MET:HB3	1:A:1151:TYR:HE1	1.55	0.72
1:A:708:VAL:HG12	1:A:788:VAL:CG1	2.20	0.72
1:A:711:VAL:HG23	1:A:711:VAL:O	1.88	0.72
1:A:504:LEU:O	1:A:508:ILE:HG13	1.90	0.71
1:A:95:GLU:OE2	1:A:100:LYS:HG3	1.90	0.71
1:A:522:LEU:HD21	1:A:1275:TRP:HZ3	1.53	0.71
1:A:1394:SER:HB3	1:A:1397:GLU:OE2	1.90	0.71
1:A:1499:LEU:CB	1:A:1504:ILE:HA	2.19	0.71
1:A:846:ILE:HD11	1:A:849:MET:CG	2.20	0.71
1:A:328:SER:HA	1:A:384:TYR:CD1	2.25	0.71
1:A:522:LEU:HD21	1:A:1275:TRP:CZ3	2.25	0.71
1:A:104:PRO:O	1:A:108:VAL:HG23	1.91	0.71
1:A:328:SER:CA	1:A:384:TYR:CE1	2.73	0.71
1:A:470:VAL:HA	1:A:473:MET:CE	2.19	0.71
1:A:1296:ASP:HA	1:A:1311:HIS:C	2.14	0.71
1:A:810:VAL:HG23	1:A:811:ILE:CG1	2.20	0.71
1:A:230:GLN:OE1	1:A:233:ARG:NH2	2.23	0.70
1:A:1294:PHE:HB2	1:A:1314:VAL:H	1.54	0.70
1:A:328:SER:CB	1:A:384:TYR:CE1	2.75	0.70
1:A:819:ASN:O	1:A:820:LYS:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TYR:HA	1:A:367:THR:HG22	1.72	0.70
1:A:792:ASP:HA	1:A:825:VAL:HG12	1.73	0.70
1:A:75:THR:HG22	1:A:79:PHE:CE2	2.26	0.70
1:A:1070:ASN:O	1:A:1074:ARG:HD3	1.91	0.70
1:A:738:LYS:O	1:A:742:GLU:HG3	1.92	0.70
1:A:636:LYS:HA	1:A:636:LYS:CE	2.17	0.69
1:A:1119:PRO:HB2	1:A:1120:PRO:HD3	1.74	0.69
1:A:1294:PHE:O	1:A:1313:ASN:HA	1.92	0.69
1:A:69:HIS:HA	1:A:72:LYS:HE2	1.74	0.69
1:A:170:PHE:O	1:A:174:THR:HG23	1.93	0.69
1:A:682:CYS:SG	1:A:684:LYS:HG3	2.32	0.69
1:A:829:ILE:HA	1:A:832:LEU:CD1	2.22	0.69
1:A:1029:VAL:HG23	1:A:1032:TYR:CE1	2.28	0.69
1:A:1123:LEU:C	1:A:1124:ILE:HD13	2.18	0.69
1:A:1308:VAL:O	1:A:1309:LEU:HD23	1.91	0.69
1:A:384:TYR:HH	1:A:442:ASN:CG	1.99	0.68
1:A:645:THR:HG22	1:A:703:THR:CG2	2.23	0.68
1:A:515:LEU:HD23	1:A:520:TRP:HB2	1.74	0.68
1:A:81:LEU:HB3	1:A:117:MET:HG3	1.74	0.68
1:A:328:SER:CA	1:A:384:TYR:CD1	2.77	0.68
1:A:1026:GLY:O	1:A:1029:VAL:HG12	1.94	0.68
1:A:1282:PRO:HG3	1:A:1360:ILE:HD11	1.74	0.68
1:A:162:LYS:HE3	1:A:162:LYS:CA	2.18	0.68
1:A:444:ILE:CD1	1:A:606:ILE:CD1	2.72	0.68
1:A:806:ILE:O	1:A:810:VAL:HG22	1.93	0.68
1:A:653:TRP:CZ2	1:A:695:MET:HE2	2.29	0.68
1:A:761:ILE:CG2	1:A:765:GLY:HA2	2.24	0.68
1:A:640:ALA:O	1:A:705:LYS:NZ	2.16	0.68
1:A:742:GLU:CA	1:A:747:LEU:HD11	2.18	0.68
1:A:1300:ARG:CB	1:A:1307:LEU:HA	2.24	0.68
1:A:444:ILE:CD1	1:A:606:ILE:HD11	2.23	0.67
1:A:10:ASP:OD1	1:A:12:SER:HB3	1.93	0.67
1:A:493:ALA:HA	1:A:496:LYS:HG2	1.75	0.67
1:A:644:ILE:HB	1:A:668:VAL:HG22	1.75	0.67
1:A:761:ILE:O	1:A:766:VAL:N	2.18	0.67
1:A:228:MET:HE1	1:A:1194:ALA:HB1	1.77	0.67
1:A:732:LEU:HD23	1:A:733:GLN:N	2.10	0.67
1:A:694:GLU:OE1	1:A:1165:ARG:NH1	2.28	0.67
1:A:746:LEU:HA	1:A:749:ASP:OD2	1.94	0.67
1:A:1390:PHE:CB	1:A:1392:GLN:HG2	2.25	0.67
1:A:1357:ILE:HA	1:A:1360:ILE:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:ARG:HA	1:A:1437:VAL:CG2	2.24	0.67
1:A:516:LYS:HE3	1:A:1272:GLU:OE2	1.95	0.66
1:A:642:ASN:ND2	1:A:667:SER:OG	2.27	0.66
1:A:853:GLN:O	1:A:856:LEU:HG	1.95	0.66
1:A:462:LEU:CD2	1:A:564:THR:CG2	2.74	0.66
1:A:801:HIS:O	1:A:804:LYS:HG3	1.95	0.66
1:A:1498:VAL:O	1:A:1505:GLN:N	2.23	0.66
1:A:327:MET:HE1	1:A:330:LEU:HD13	1.75	0.66
1:A:1495:ARG:NH2	1:A:1507:TRP:HB2	2.08	0.66
1:A:839:ILE:HG22	1:A:849:MET:CG	2.26	0.66
1:A:717:ILE:HD12	1:A:761:ILE:HG21	1.77	0.66
1:A:642:ASN:OD1	1:A:669:PRO:HA	1.96	0.66
1:A:1117:ILE:HG21	1:A:1212:PHE:CD2	2.31	0.66
1:A:635:ILE:HG23	1:A:636:LYS:HD2	1.79	0.65
1:A:405:ARG:HG3	1:A:405:ARG:HH11	1.60	0.65
1:A:793:ASP:OD1	1:A:796:SER:HB2	1.96	0.65
1:A:57:LEU:O	1:A:130:ARG:HD2	1.97	0.65
1:A:719:ASN:ND2	1:A:764:LYS:HA	2.10	0.65
1:A:444:ILE:HD11	1:A:606:ILE:HD12	1.77	0.65
1:A:455:LEU:HD21	1:A:473:MET:HE1	1.79	0.65
1:A:1282:PRO:CG	1:A:1360:ILE:HD11	2.26	0.65
1:A:69:HIS:HA	1:A:72:LYS:CE	2.27	0.65
1:A:470:VAL:HA	1:A:473:MET:HE3	1.79	0.65
1:A:473:MET:HG2	1:A:596:LEU:CD1	2.27	0.65
1:A:1310:LYS:N	1:A:1502:GLY:O	2.29	0.65
1:A:15:PHE:O	1:A:30:THR:HG21	1.97	0.64
1:A:825:VAL:HG13	1:A:825:VAL:O	1.97	0.64
1:A:1496:VAL:C	1:A:1497:ILE:HD12	2.22	0.64
1:A:515:LEU:HD21	1:A:524:PHE:CE2	2.33	0.64
1:A:1199:ALA:O	1:A:1203:GLU:HG2	1.97	0.64
1:A:490:TYR:CE2	1:A:541:LYS:HB3	2.32	0.64
1:A:261:TRP:HE3	1:A:316:VAL:HG21	1.63	0.64
1:A:1044:SER:HB2	1:A:1083:ASP:OD2	1.98	0.64
1:A:357:LYS:HE3	1:A:357:LYS:HA	1.79	0.64
1:A:1340:PHE:CZ	1:A:1371:ILE:HB	2.33	0.64
1:A:1437:VAL:O	1:A:1441:ARG:HG3	1.98	0.64
1:A:839:ILE:HG22	1:A:849:MET:HG2	1.79	0.63
1:A:840:VAL:HG23	1:A:847:SER:HB3	1.78	0.63
1:A:1451:VAL:HG13	1:A:1481:LEU:O	1.98	0.63
1:A:1117:ILE:HD12	1:A:1212:PHE:CE2	2.33	0.63
1:A:462:LEU:CD2	1:A:564:THR:HG21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LEU:HB2	1:A:748:PRO:HD3	1.81	0.63
1:A:676:VAL:CG1	1:A:825:VAL:HG23	2.27	0.63
1:A:104:PRO:O	1:A:107:LEU:HG	1.99	0.63
1:A:67:MET:SD	1:A:128:ARG:NH1	2.71	0.63
1:A:162:LYS:HA	1:A:162:LYS:CE	2.20	0.63
1:A:409:VAL:CG1	1:A:624:ASP:HB3	2.28	0.63
1:A:232:TYR:OH	1:A:1130:ARG:NH2	2.32	0.63
1:A:467:LEU:HA	1:A:470:VAL:CG1	2.27	0.63
1:A:1148:SER:OG	1:A:1149:PRO:HD3	1.98	0.63
1:A:1308:VAL:O	1:A:1308:VAL:HG12	1.98	0.63
1:A:1397:GLU:OE1	1:A:1397:GLU:N	2.17	0.63
1:A:1517:ARG:HA	1:A:1521:TYR:CB	2.29	0.63
1:A:427:MET:HB3	1:A:1151:TYR:CE1	2.32	0.62
1:A:653:TRP:CE2	1:A:695:MET:HE2	2.33	0.62
1:A:1382:SER:O	1:A:1385:MET:HG3	1.98	0.62
1:A:1299:LEU:HA	1:A:1346:ALA:CB	2.30	0.62
1:A:1029:VAL:HG23	1:A:1032:TYR:HE1	1.63	0.62
1:A:677:VAL:O	1:A:840:VAL:HA	1.99	0.62
1:A:860:GLY:O	1:A:863:ALA:HB3	1.98	0.62
1:A:1388:ASP:OD2	1:A:1393:TYR:N	2.28	0.62
1:A:6:PHE:CE1	1:A:104:PRO:HB2	2.35	0.62
1:A:30:THR:O	1:A:34:GLN:HG3	1.98	0.62
1:A:1099:ASN:HB3	1:A:1242:TYR:CD2	2.35	0.62
1:A:1497:ILE:HA	1:A:1506:GLU:O	2.00	0.62
1:A:673:LEU:HB2	1:A:822:ARG:NH2	2.15	0.61
1:A:493:ALA:HA	1:A:496:LYS:HZ2	1.65	0.61
1:A:6:PHE:O	1:A:104:PRO:HD2	2.00	0.61
1:A:261:TRP:CH2	1:A:311:PRO:HB2	2.35	0.61
1:A:1322:VAL:HG13	1:A:1495:ARG:C	2.25	0.61
1:A:127:GLU:O	1:A:132:VAL:HG12	1.99	0.61
1:A:708:VAL:HG12	1:A:788:VAL:HG11	1.83	0.61
1:A:507:GLU:CD	1:A:1379:PHE:HD1	2.08	0.61
1:A:328:SER:HA	1:A:384:TYR:HD1	1.63	0.61
1:A:338:MET:HE1	1:A:373:SER:HA	1.82	0.61
1:A:852:TYR:CD1	1:A:856:LEU:HD23	2.36	0.61
1:A:261:TRP:CE3	1:A:316:VAL:HG21	2.36	0.61
1:A:264:GLU:HG3	1:A:316:VAL:CG2	2.31	0.61
1:A:467:LEU:CA	1:A:470:VAL:HG12	2.30	0.61
1:A:164:ASP:O	1:A:166:ARG:NH1	2.34	0.60
1:A:66:GLN:HG2	1:A:67:MET:N	2.16	0.60
1:A:1486:ARG:O	1:A:1489:THR:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:HB1	1:A:104:PRO:CD	2.32	0.60
1:A:1099:ASN:HB3	1:A:1242:TYR:CE2	2.37	0.60
1:A:1407:LEU:HG	1:A:1407:LEU:O	2.00	0.60
1:A:74:LYS:HB3	1:A:124:ILE:HD13	1.84	0.60
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.84	0.60
1:A:473:MET:HG2	1:A:596:LEU:HD11	1.84	0.59
1:A:1495:ARG:HA	1:A:1509:SER:HA	1.84	0.59
1:A:444:ILE:CG1	1:A:606:ILE:HD11	2.32	0.59
1:A:1198:LEU:HD11	1:A:1247:VAL:HG11	1.82	0.59
1:A:1282:PRO:CG	1:A:1364:ASP:HB3	2.25	0.59
1:A:1352:ILE:HG22	1:A:1353:ASP:OD2	2.02	0.59
1:A:790:LEU:CD2	1:A:823:LEU:HD12	2.32	0.59
1:A:156:LYS:HD3	1:A:172:ASP:OD2	2.02	0.59
1:A:467:LEU:HD23	1:A:470:VAL:HG11	1.84	0.59
1:A:688:LEU:HD12	1:A:792:ASP:CB	2.32	0.59
1:A:1255:THR:O	1:A:1258:VAL:HG22	2.02	0.59
1:A:1289:VAL:O	1:A:1318:GLY:HA3	2.02	0.59
1:A:1294:PHE:HB2	1:A:1314:VAL:N	2.18	0.59
1:A:1177:SER:O	1:A:1181:VAL:HG23	2.02	0.59
1:A:1278:GLN:HA	1:A:1281:ALA:HB2	1.84	0.59
1:A:832:LEU:H	1:A:832:LEU:HD12	1.67	0.59
1:A:1060:ILE:HG13	1:A:1342:ILE:CG2	2.31	0.59
1:A:499:ASP:C	1:A:502:ILE:HG22	2.27	0.59
1:A:632:ARG:O	1:A:633:ARG:HG3	2.03	0.59
1:A:807:PHE:O	1:A:812:GLY:N	2.32	0.59
1:A:841:MET:HA	1:A:847:SER:N	2.13	0.59
1:A:483:MET:HE3	1:A:548:VAL:HG11	1.84	0.59
1:A:1365:LEU:HD21	1:A:1369:ILE:HD12	1.85	0.59
1:A:614:LYS:O	1:A:618:VAL:HG23	2.03	0.58
1:A:435:MET:HE2	1:A:1188:TYR:CZ	2.38	0.58
1:A:654:ALA:HB3	1:A:657:ASP:OD1	2.02	0.58
1:A:367:THR:OG1	1:A:1211:LEU:HD12	2.02	0.58
1:A:800:ALA:O	1:A:804:LYS:HG2	2.03	0.58
1:A:708:VAL:HG23	1:A:1166:ALA:O	2.02	0.58
1:A:810:VAL:CG2	1:A:811:ILE:HG13	2.30	0.58
1:A:593:ARG:HG3	1:A:594:PHE:N	2.17	0.58
1:A:630:ILE:HD11	1:A:690:ALA:O	2.04	0.58
1:A:162:LYS:HB3	1:A:164:ASP:OD2	2.04	0.58
1:A:866:LEU:HD12	1:A:870:ALA:CB	2.33	0.58
1:A:75:THR:HG22	1:A:79:PHE:HE2	1.69	0.58
1:A:364:TYR:OH	1:A:1219:ILE:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:O	1:A:986:VAL:HG23	2.04	0.57
1:A:744:CYS:O	1:A:775:ARG:HD2	2.04	0.57
1:A:722:LEU:HD13	1:A:768:LEU:HD11	1.86	0.57
1:A:78:GLY:HA3	1:A:121:THR:HG22	1.86	0.57
1:A:761:ILE:HG23	1:A:765:GLY:HA2	1.87	0.57
1:A:7:CYS:HA	1:A:105:VAL:HG11	1.85	0.57
1:A:750:LEU:HA	1:A:753:LEU:CG	2.34	0.57
1:A:1185:GLN:OE1	1:A:1185:GLN:HA	2.05	0.57
1:A:1449:ILE:HG22	1:A:1479:THR:CB	2.24	0.57
1:A:169:VAL:O	1:A:173:VAL:HG23	2.05	0.57
1:A:410:ILE:HD11	1:A:619:PHE:CZ	2.40	0.57
1:A:809:ASN:O	1:A:816:LEU:N	2.35	0.57
1:A:1331:GLY:O	1:A:1334:SER:N	2.37	0.57
1:A:717:ILE:HG13	1:A:717:ILE:O	2.02	0.57
1:A:375:CYS:HA	1:A:378:THR:HG22	1.87	0.57
1:A:718:GLN:HG2	1:A:1156:GLU:OE2	2.04	0.57
1:A:1360:ILE:HG13	1:A:1361:GLY:N	2.19	0.57
1:A:105:VAL:HG13	1:A:106:PHE:CD1	2.39	0.57
1:A:499:ASP:HA	1:A:502:ILE:HG22	1.87	0.57
1:A:516:LYS:HG3	1:A:1060:ILE:HD11	1.87	0.57
1:A:30:THR:HG23	1:A:33:PHE:H	1.69	0.57
1:A:647:LYS:NZ	1:A:648:ASN:HB2	2.20	0.57
1:A:676:VAL:HG23	1:A:839:ILE:HG13	1.87	0.57
1:A:1291:ARG:O	1:A:1352:ILE:HG23	2.05	0.57
1:A:1371:ILE:CD1	1:A:1451:VAL:HB	2.34	0.57
1:A:1371:ILE:HD12	1:A:1451:VAL:HB	1.85	0.57
1:A:753:LEU:HD12	1:A:756:GLY:H	1.70	0.56
1:A:375:CYS:O	1:A:378:THR:HG22	2.05	0.56
1:A:633:ARG:NH2	1:A:639:GLY:HA3	2.20	0.56
1:A:168:ASP:OD1	1:A:170:PHE:N	2.37	0.56
1:A:493:ALA:CA	1:A:496:LYS:HZ2	2.18	0.56
1:A:769:SER:O	1:A:772:GLN:N	2.39	0.56
1:A:866:LEU:HD12	1:A:870:ALA:HB3	1.87	0.56
1:A:572:ASP:OD1	1:A:574:ASN:N	2.39	0.56
1:A:1121:LEU:HD21	1:A:1205:VAL:HG13	1.87	0.56
1:A:156:LYS:HA	1:A:159:THR:HG22	1.88	0.56
1:A:747:LEU:HD12	1:A:747:LEU:H	1.70	0.56
1:A:819:ASN:C	1:A:820:LYS:HD3	2.31	0.56
1:A:1343:LYS:HD3	1:A:1343:LYS:C	2.30	0.56
1:A:435:MET:HE2	1:A:1188:TYR:CE2	2.40	0.56
1:A:594:PHE:HB3	1:A:595:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:HH22	1:A:708:VAL:CG1	2.19	0.56
1:A:1119:PRO:CB	1:A:1120:PRO:HD3	2.36	0.56
1:A:1299:LEU:H	1:A:1309:LEU:HG	1.71	0.56
1:A:711:VAL:HG22	1:A:791:LEU:HA	1.86	0.56
1:A:861:ALA:O	1:A:864:GLU:N	2.39	0.56
1:A:471:ALA:O	1:A:474:VAL:HG12	2.05	0.56
1:A:668:VAL:CG1	1:A:674:VAL:HG21	2.29	0.56
1:A:62:ARG:NH2	1:A:133:GLN:HG3	2.20	0.55
1:A:1448:LYS:O	1:A:1478:CYS:HA	2.06	0.55
1:A:81:LEU:HD21	1:A:181:LEU:HB3	1.87	0.55
1:A:789:TYR:HB3	1:A:791:LEU:CD1	2.36	0.55
1:A:1308:VAL:C	1:A:1309:LEU:HD23	2.32	0.55
1:A:1362:LEU:HD22	1:A:1366:ARG:HH21	1.71	0.55
1:A:19:ASN:HB3	2:A:1601:NAG:N2	2.21	0.55
1:A:636:LYS:HE3	1:A:636:LYS:CA	2.22	0.55
1:A:655:ARG:HG3	1:A:656:ASN:ND2	2.21	0.55
1:A:778:LEU:HD21	1:A:810:VAL:HG21	1.89	0.55
1:A:840:VAL:O	1:A:847:SER:N	2.38	0.55
1:A:1351:ILE:HA	1:A:1355:ILE:O	2.05	0.55
1:A:1398:VAL:O	1:A:1401:SER:OG	2.25	0.55
1:A:16:TRP:CE2	1:A:21:THR:HG21	2.42	0.55
1:A:726:ILE:HD11	1:A:746:LEU:HD11	1.89	0.55
1:A:958:LYS:O	1:A:960:SER:N	2.40	0.55
1:A:1198:LEU:CD1	1:A:1247:VAL:HG11	2.35	0.55
1:A:1362:LEU:O	1:A:1366:ARG:HG3	2.07	0.55
1:A:1233:VAL:O	1:A:1237:LEU:HD13	2.05	0.55
1:A:1287:PRO:HG3	1:A:1368:LYS:CB	2.37	0.55
1:A:462:LEU:HD23	1:A:564:THR:HG21	1.89	0.55
1:A:1292:VAL:O	1:A:1316:ILE:N	2.35	0.55
1:A:1422:CYS:SG	1:A:1423:ALA:N	2.80	0.55
1:A:78:GLY:HA3	1:A:121:THR:CG2	2.37	0.55
1:A:646:VAL:HG12	1:A:702:VAL:CG2	2.30	0.55
1:A:1060:ILE:CG1	1:A:1342:ILE:HG23	2.37	0.55
1:A:573:GLU:CD	1:A:573:GLU:H	2.15	0.55
1:A:851:SER:HB3	1:A:854:GLU:OE1	2.06	0.55
1:A:4:ARG:O	1:A:11:GLY:HA2	2.07	0.55
1:A:6:PHE:HA	1:A:104:PRO:HD2	1.88	0.55
1:A:107:LEU:C	1:A:107:LEU:HD12	2.32	0.55
1:A:467:LEU:O	1:A:470:VAL:HG12	2.08	0.54
1:A:515:LEU:HD11	1:A:524:PHE:CE2	2.42	0.54
1:A:1382:SER:O	1:A:1385:MET:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD21	1:A:181:LEU:CB	2.37	0.54
1:A:62:ARG:HH22	1:A:133:GLN:HG3	1.72	0.54
1:A:228:MET:CE	1:A:1194:ALA:HB1	2.36	0.54
1:A:666:PHE:HA	1:A:849:MET:HE1	1.90	0.54
1:A:1202:LEU:HD11	1:A:1247:VAL:HG21	1.89	0.54
1:A:520:TRP:CD2	1:A:1389:PRO:HG3	2.42	0.54
1:A:1361:GLY:O	1:A:1364:ASP:N	2.39	0.54
1:A:109:SER:HB3	1:A:110:PRO:HD3	1.88	0.54
1:A:153:LEU:HD11	1:A:157:ILE:HD11	1.90	0.54
1:A:647:LYS:HZ2	1:A:648:ASN:HB2	1.73	0.54
1:A:652:THR:HB	1:A:659:PRO:HA	1.88	0.54
1:A:462:LEU:HG	1:A:462:LEU:O	2.07	0.54
1:A:774:GLN:HG3	1:A:797:ALA:HB3	1.89	0.54
1:A:795:LEU:HD12	1:A:795:LEU:H	1.73	0.54
1:A:1394:SER:HB3	1:A:1397:GLU:CD	2.33	0.54
1:A:405:ARG:HG3	1:A:405:ARG:NH1	2.24	0.53
1:A:721:SER:O	1:A:724:GLU:N	2.41	0.53
1:A:961:VAL:HG12	1:A:1257:ILE:HG13	1.90	0.53
1:A:345:ILE:HB	1:A:370:LEU:HD13	1.90	0.53
1:A:163:GLU:C	1:A:166:ARG:HH22	2.16	0.53
1:A:410:ILE:HG23	1:A:414:ALA:CB	2.25	0.53
1:A:630:ILE:HG23	1:A:702:VAL:CG1	2.34	0.53
1:A:983:CYS:HB3	1:A:1028:THR:HG21	1.90	0.53
1:A:1382:SER:HA	1:A:1421:GLU:CA	2.31	0.53
1:A:361:TRP:HA	1:A:364:TYR:HD2	1.74	0.53
1:A:382:HIS:CE1	1:A:1199:ALA:HB1	2.44	0.53
1:A:520:TRP:HH2	1:A:1441:ARG:HH11	1.55	0.53
1:A:664:ILE:HG21	1:A:666:PHE:HE1	1.74	0.53
1:A:234:GLN:HB2	1:A:235:PRO:HD2	1.91	0.53
1:A:1123:LEU:O	1:A:1124:ILE:HD13	2.09	0.53
1:A:41:VAL:HB	1:A:42:PRO:HD3	1.90	0.53
1:A:94:TRP:O	1:A:98:MET:HB2	2.08	0.53
1:A:673:LEU:O	1:A:836:ASP:HB3	2.08	0.53
1:A:829:ILE:HA	1:A:832:LEU:HD13	1.90	0.53
1:A:692:LEU:HD11	1:A:710:TYR:CG	2.44	0.53
1:A:327:MET:HE3	1:A:327:MET:HA	1.91	0.52
1:A:338:MET:CE	1:A:373:SER:HA	2.38	0.52
1:A:444:ILE:CD1	1:A:602:VAL:HG12	2.38	0.52
1:A:582:ALA:O	1:A:583:PHE:HB2	2.09	0.52
1:A:1384:ARG:HB2	1:A:1418:LEU:O	2.09	0.52
1:A:477:VAL:CG2	1:A:478:PRO:HD3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:GLU:HA	1:A:1315:THR:HA	1.90	0.52
1:A:543:ALA:HB1	1:A:1037:SER:HB3	1.91	0.52
1:A:1117:ILE:C	1:A:1120:PRO:HD2	2.33	0.52
1:A:521:GLU:OE2	1:A:1363:HIS:HE1	1.92	0.52
1:A:1117:ILE:HD12	1:A:1212:PHE:CZ	2.45	0.52
1:A:676:VAL:HA	1:A:839:ILE:O	2.10	0.52
1:A:716:TRP:CZ3	1:A:1163:VAL:HB	2.44	0.52
1:A:327:MET:O	1:A:331:PHE:HD2	1.93	0.52
1:A:1361:GLY:HA3	1:A:1364:ASP:OD2	2.10	0.52
1:A:507:GLU:OE2	1:A:1379:PHE:HD1	1.92	0.52
1:A:1322:VAL:O	1:A:1481:LEU:HA	2.10	0.52
1:A:683:GLY:C	1:A:841:MET:HE1	2.35	0.52
1:A:85:CYS:SG	1:A:113:LEU:HD23	2.50	0.52
1:A:357:LYS:HE3	1:A:357:LYS:CA	2.40	0.51
1:A:738:LYS:O	1:A:741:VAL:HG12	2.10	0.51
1:A:957:VAL:HG23	1:A:957:VAL:O	2.10	0.51
1:A:183:LEU:O	1:A:187:VAL:HG23	2.10	0.51
1:A:484:ALA:O	1:A:487:THR:HG22	2.11	0.51
1:A:504:LEU:CD2	1:A:527:LYS:HG2	2.40	0.51
1:A:508:ILE:HG23	1:A:515:LEU:HD13	1.91	0.51
1:A:346:LEU:HD13	1:A:1233:VAL:HG11	1.93	0.51
1:A:467:LEU:CD2	1:A:470:VAL:HG11	2.40	0.51
1:A:470:VAL:HA	1:A:473:MET:HE2	1.90	0.51
1:A:474:VAL:O	1:A:477:VAL:HG22	2.10	0.51
1:A:516:LYS:HG3	1:A:1060:ILE:CD1	2.39	0.51
1:A:650:THR:HG22	1:A:662:HIS:HA	1.92	0.51
1:A:666:PHE:CB	1:A:849:MET:HE1	2.39	0.51
1:A:958:LYS:C	1:A:960:SER:H	2.19	0.51
1:A:1369:ILE:HG12	1:A:1449:ILE:HD11	1.92	0.51
1:A:332:LYS:HB2	1:A:384:TYR:CZ	2.46	0.51
1:A:741:VAL:HG23	1:A:746:LEU:HD12	1.93	0.51
1:A:1434:ARG:HA	1:A:1437:VAL:HG23	1.91	0.51
1:A:14:LEU:HD12	1:A:14:LEU:H	1.75	0.51
1:A:384:TYR:HH	1:A:442:ASN:CB	2.23	0.51
1:A:518:TYR:O	1:A:519:ALA:HB3	2.10	0.51
1:A:163:GLU:N	1:A:163:GLU:OE1	2.43	0.51
1:A:1171:GLU:OE2	1:A:1171:GLU:HA	2.10	0.51
1:A:56:TYR:HD1	1:A:57:LEU:HD12	1.75	0.51
1:A:364:TYR:HA	1:A:367:THR:CG2	2.39	0.51
1:A:477:VAL:HG23	1:A:478:PRO:HD3	1.92	0.51
1:A:676:VAL:HA	1:A:839:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD23	1:A:520:TRP:CB	2.40	0.51
1:A:1189:TYR:HB3	1:A:1190:PRO:HD3	1.92	0.51
1:A:586:LEU:HD11	1:A:995:LEU:HD23	1.93	0.50
1:A:769:SER:H	1:A:772:GLN:HG3	1.75	0.50
1:A:544:TYR:HD1	1:A:1034:MET:SD	2.34	0.50
1:A:647:LYS:HZ2	1:A:648:ASN:CB	2.24	0.50
1:A:1175:ARG:HB3	1:A:1175:ARG:NH1	2.26	0.50
1:A:757:ASP:OD1	1:A:758:ARG:N	2.45	0.50
1:A:805:HIS:O	1:A:808:GLU:HG3	2.11	0.50
1:A:1181:VAL:O	1:A:1185:GLN:HG2	2.12	0.50
1:A:82:TRP:CD1	1:A:118:LEU:HG	2.47	0.50
1:A:666:PHE:HB3	1:A:849:MET:HE1	1.92	0.50
1:A:1362:LEU:HD22	1:A:1366:ARG:HE	1.76	0.50
1:A:20:VAL:HG12	1:A:28:ASP:O	2.11	0.49
1:A:1215:LEU:O	1:A:1219:ILE:HG12	2.12	0.49
1:A:173:VAL:O	1:A:177:ILE:HG12	2.12	0.49
1:A:645:THR:HG22	1:A:703:THR:HG22	1.91	0.49
1:A:811:ILE:O	1:A:822:ARG:NH1	2.45	0.49
1:A:443:MET:HE2	1:A:594:PHE:HE2	1.78	0.49
1:A:664:ILE:HG22	1:A:666:PHE:CD1	2.47	0.49
1:A:745:ALA:O	1:A:749:ASP:OD2	2.30	0.49
1:A:1215:LEU:O	1:A:1215:LEU:HD23	2.12	0.49
1:A:477:VAL:N	1:A:478:PRO:HD2	2.28	0.49
1:A:648:ASN:OD1	1:A:663:GLY:HA2	2.13	0.49
1:A:839:ILE:CG2	1:A:849:MET:SD	3.00	0.49
1:A:1245:TRP:HA	1:A:1245:TRP:CE3	2.48	0.49
1:A:1275:TRP:HB3	1:A:1363:HIS:HD2	1.77	0.49
1:A:1470:THR:O	1:A:1474:GLN:N	2.45	0.49
1:A:961:VAL:CG1	1:A:1257:ILE:HG13	2.43	0.49
1:A:1317:ASP:O	1:A:1320:GLU:HG3	2.12	0.49
1:A:55:LEU:C	1:A:55:LEU:HD23	2.38	0.49
1:A:95:GLU:HG3	1:A:100:LYS:HB2	1.95	0.49
1:A:253:VAL:HG12	1:A:398:ALA:HB2	1.95	0.49
1:A:396:LYS:HD2	1:A:435:MET:SD	2.52	0.49
1:A:790:LEU:HD22	1:A:823:LEU:HD12	1.94	0.49
1:A:1005:ASN:O	1:A:1007:THR:HG22	2.11	0.49
1:A:1351:ILE:C	1:A:1352:ILE:HD12	2.38	0.49
1:A:1370:THR:HG23	1:A:1447:THR:CB	2.42	0.49
1:A:1374:GLN:N	1:A:1453:ASP:OD2	2.45	0.49
1:A:328:SER:C	1:A:384:TYR:CD1	2.77	0.49
1:A:340:PHE:CE1	1:A:591:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ILE:HG13	1:A:606:ILE:HD11	1.93	0.49
1:A:493:ALA:HB1	1:A:496:LYS:NZ	2.27	0.49
1:A:525:LYS:O	1:A:528:VAL:HG12	2.12	0.49
1:A:667:SER:O	1:A:669:PRO:HD3	2.12	0.49
1:A:722:LEU:CD1	1:A:761:ILE:HD11	2.42	0.49
1:A:846:ILE:HD11	1:A:849:MET:HG2	1.94	0.49
1:A:1175:ARG:HB3	1:A:1175:ARG:CZ	2.42	0.49
1:A:489:THR:O	1:A:492:VAL:HG12	2.13	0.49
1:A:791:LEU:HD22	1:A:811:ILE:HD13	1.94	0.49
1:A:507:GLU:OE2	1:A:1379:PHE:CD1	2.66	0.48
1:A:675:ALA:HA	1:A:824:LEU:O	2.13	0.48
1:A:1467:ILE:HA	1:A:1470:THR:OG1	2.12	0.48
1:A:633:ARG:NH2	1:A:637:ASP:OD2	2.46	0.48
1:A:1299:LEU:CA	1:A:1346:ALA:HB3	2.37	0.48
1:A:66:GLN:HG2	1:A:67:MET:H	1.77	0.48
1:A:692:LEU:HD11	1:A:710:TYR:CD1	2.48	0.48
1:A:1497:ILE:HG13	1:A:1507:TRP:HA	1.94	0.48
1:A:493:ALA:HA	1:A:496:LYS:NZ	2.27	0.48
1:A:1065:ARG:NH1	1:A:1065:ARG:HB2	2.28	0.48
1:A:1495:ARG:HH21	1:A:1508:GLY:H	1.61	0.48
1:A:1503:GLU:O	1:A:1503:GLU:HG2	2.13	0.48
1:A:257:LEU:HD12	1:A:257:LEU:O	2.14	0.48
1:A:593:ARG:CG	1:A:594:PHE:N	2.77	0.48
1:A:666:PHE:HB3	1:A:849:MET:CE	2.44	0.48
1:A:839:ILE:HG22	1:A:849:MET:SD	2.53	0.48
1:A:1385:MET:SD	1:A:1386:ASN:N	2.86	0.48
1:A:673:LEU:HD12	1:A:822:ARG:O	2.13	0.48
1:A:365:PHE:O	1:A:369:LEU:HD13	2.13	0.48
1:A:508:ILE:HD13	1:A:524:PHE:HB3	1.95	0.48
1:A:515:LEU:HD11	1:A:524:PHE:CD2	2.49	0.48
1:A:852:TYR:CE1	1:A:856:LEU:HD23	2.49	0.48
1:A:684:LYS:HB3	1:A:825:VAL:CG2	2.44	0.48
1:A:736:TYR:O	1:A:740:VAL:HG12	2.14	0.48
1:A:15:PHE:O	1:A:30:THR:CG2	2.62	0.47
1:A:702:VAL:HG22	1:A:703:THR:N	2.29	0.47
1:A:1076:SER:OG	1:A:1077:LYS:N	2.46	0.47
1:A:9:VAL:HG13	1:A:10:ASP:N	2.29	0.47
1:A:254:VAL:O	1:A:258:VAL:HG23	2.14	0.47
1:A:644:ILE:HB	1:A:668:VAL:CG2	2.44	0.47
1:A:1240:THR:HG23	1:A:1241:THR:HG23	1.96	0.47
1:A:1451:VAL:HG12	1:A:1452:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD23	1:A:181:LEU:HD23	1.97	0.47
1:A:495:MET:HA	1:A:498:LYS:HG2	1.95	0.47
1:A:648:ASN:N	1:A:664:ILE:O	2.44	0.47
1:A:831:TYR:C	1:A:833:PRO:HD2	2.39	0.47
1:A:16:TRP:CZ2	1:A:21:THR:HG21	2.50	0.47
1:A:1127:PHE:CD2	1:A:1130:ARG:HD2	2.49	0.47
1:A:1308:VAL:O	1:A:1308:VAL:CG1	2.62	0.47
1:A:504:LEU:HD21	1:A:527:LYS:HG2	1.95	0.47
1:A:795:LEU:HD23	1:A:806:ILE:HB	1.96	0.47
1:A:1119:PRO:HB2	1:A:1120:PRO:CD	2.43	0.47
1:A:62:ARG:HB2	1:A:131:GLY:O	2.15	0.47
1:A:829:ILE:HA	1:A:832:LEU:HD11	1.95	0.47
1:A:1062:PHE:CE1	1:A:1066:THR:HG21	2.50	0.47
1:A:1340:PHE:HZ	1:A:1371:ILE:HB	1.79	0.47
1:A:1372:ILE:HD11	1:A:1442:ALA:CB	2.45	0.47
1:A:18:TRP:HE3	1:A:22:TRP:HB3	1.78	0.47
1:A:44:SER:O	1:A:48:VAL:HG12	2.15	0.47
1:A:164:ASP:OD2	1:A:164:ASP:N	2.45	0.47
1:A:716:TRP:HE3	1:A:1163:VAL:HG21	1.79	0.47
1:A:728:PHE:CD1	1:A:780:ARG:HD2	2.49	0.47
1:A:1292:VAL:O	1:A:1315:THR:HA	2.14	0.47
1:A:1357:ILE:CA	1:A:1360:ILE:HG22	2.41	0.47
1:A:84:VAL:HG22	1:A:84:VAL:O	2.15	0.47
1:A:419:THR:OG1	1:A:422:GLU:HG3	2.14	0.47
1:A:665:THR:O	1:A:849:MET:HE1	2.15	0.47
1:A:1357:ILE:HA	1:A:1360:ILE:CG2	2.42	0.47
1:A:429:VAL:HG23	1:A:430:ASP:N	2.29	0.47
1:A:664:ILE:HG22	1:A:666:PHE:HD1	1.80	0.47
1:A:434:PHE:CZ	1:A:613:LEU:HB2	2.50	0.47
1:A:451:VAL:HA	1:A:592:LEU:HD11	1.97	0.47
1:A:794:PRO:HG2	1:A:795:LEU:CD1	2.44	0.47
1:A:801:HIS:NE2	1:A:805:HIS:NE2	2.63	0.47
1:A:1441:ARG:O	1:A:1445:ARG:HG2	2.15	0.47
1:A:31:LYS:HE3	1:A:34:GLN:NE2	2.30	0.46
1:A:68:THR:HG22	1:A:71:ASN:HD21	1.77	0.46
1:A:375:CYS:O	1:A:378:THR:CG2	2.63	0.46
1:A:499:ASP:O	1:A:502:ILE:CG2	2.56	0.46
1:A:665:THR:O	1:A:849:MET:CE	2.62	0.46
1:A:666:PHE:CA	1:A:849:MET:HE1	2.45	0.46
1:A:846:ILE:HG23	1:A:846:ILE:O	2.15	0.46
1:A:493:ALA:CB	1:A:496:LYS:NZ	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:PHE:HB3	1:A:695:MET:SD	2.55	0.46
1:A:594:PHE:CZ	1:A:598:ILE:HG13	2.50	0.46
1:A:1371:ILE:HG13	1:A:1373:PRO:HD3	1.97	0.46
1:A:6:PHE:O	1:A:105:VAL:HG12	2.15	0.46
1:A:458:LEU:O	1:A:462:LEU:HB3	2.15	0.46
1:A:1316:ILE:HG23	1:A:1320:GLU:CD	2.40	0.46
1:A:486:LYS:HA	1:A:489:THR:HB	1.97	0.46
1:A:515:LEU:HD21	1:A:524:PHE:CZ	2.51	0.46
1:A:969:ILE:HG23	1:A:1039:GLY:HA3	1.97	0.46
1:A:434:PHE:HZ	1:A:613:LEU:HB2	1.80	0.46
1:A:513:LYS:HE2	1:A:513:LYS:HB3	1.71	0.46
1:A:1044:SER:HB2	1:A:1083:ASP:CG	2.41	0.46
1:A:1048:HIS:HB2	1:A:1079:LEU:HD21	1.96	0.46
1:A:82:TRP:CE3	1:A:83:ILE:HG13	2.51	0.46
1:A:487:THR:HG23	1:A:488:LYS:N	2.30	0.46
1:A:841:MET:HB2	1:A:841:MET:HE3	1.85	0.46
1:A:1357:ILE:C	1:A:1360:ILE:HG22	2.41	0.46
1:A:332:LYS:HB2	1:A:384:TYR:CE1	2.51	0.46
1:A:352:PHE:CZ	1:A:1221:ARG:HD3	2.46	0.46
1:A:1203:GLU:OE1	1:A:1240:THR:OG1	2.34	0.46
1:A:36:THR:HB	1:A:40:TRP:CZ3	2.50	0.46
1:A:550:THR:HG21	1:A:1033:SER:OG	2.14	0.46
1:A:694:GLU:OE1	1:A:694:GLU:HA	2.16	0.46
1:A:1336:THR:OG1	1:A:1337:LEU:N	2.49	0.46
1:A:1362:LEU:HD22	1:A:1366:ARG:NH2	2.29	0.46
1:A:1434:ARG:HA	1:A:1437:VAL:HG21	1.97	0.46
1:A:594:PHE:CE1	1:A:598:ILE:HG13	2.51	0.46
1:A:630:ILE:HG12	1:A:702:VAL:HG11	1.97	0.46
1:A:732:LEU:HD23	1:A:732:LEU:C	2.40	0.46
1:A:105:VAL:HG13	1:A:106:PHE:N	2.31	0.45
1:A:249:THR:O	1:A:253:VAL:HG23	2.15	0.45
1:A:741:VAL:HG23	1:A:746:LEU:CB	2.45	0.45
1:A:825:VAL:O	1:A:825:VAL:CG1	2.63	0.45
1:A:529:LEU:O	1:A:533:GLN:HG2	2.16	0.45
1:A:9:VAL:HG13	1:A:10:ASP:H	1.82	0.45
1:A:664:ILE:HG21	1:A:666:PHE:CE1	2.50	0.45
1:A:753:LEU:HD12	1:A:753:LEU:O	2.16	0.45
1:A:1276:GLN:NE2	1:A:1363:HIS:HB2	2.12	0.45
1:A:7:CYS:HA	1:A:105:VAL:CG1	2.45	0.45
1:A:1132:TYR:O	1:A:1133:VAL:C	2.58	0.45
1:A:1292:VAL:N	1:A:1316:ILE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:VAL:HG22	1:A:1494:THR:HG1	1.82	0.45
1:A:260:ASN:HB3	1:A:316:VAL:HG13	1.98	0.45
1:A:633:ARG:NE	1:A:637:ASP:OD1	2.47	0.45
1:A:1336:THR:O	1:A:1339:LEU:N	2.49	0.45
1:A:1372:ILE:HD11	1:A:1442:ALA:HB2	1.99	0.45
1:A:335:HIS:HE1	1:A:377:GLN:HE21	1.63	0.45
1:A:558:PHE:CE1	1:A:1022:GLY:HA3	2.50	0.45
1:A:473:MET:SD	1:A:596:LEU:HD11	2.57	0.45
1:A:976:LEU:HD12	1:A:976:LEU:HA	1.81	0.45
1:A:1077:LYS:N	1:A:1077:LYS:HD3	2.32	0.45
1:A:1103:ALA:CB	1:A:1239:VAL:HG22	2.47	0.45
1:A:225:THR:O	1:A:229:VAL:HG23	2.17	0.45
1:A:364:TYR:CA	1:A:367:THR:HG22	2.45	0.45
1:A:710:TYR:CD2	1:A:712:PRO:HD3	2.52	0.45
1:A:335:HIS:ND1	1:A:377:GLN:HG3	2.31	0.45
1:A:630:ILE:HG12	1:A:702:VAL:CG1	2.47	0.45
1:A:646:VAL:CG1	1:A:702:VAL:HG23	2.31	0.45
1:A:684:LYS:HB3	1:A:825:VAL:HG21	1.99	0.45
1:A:1370:THR:OG1	1:A:1450:LEU:HA	2.17	0.45
1:A:467:LEU:C	1:A:470:VAL:HG12	2.41	0.44
1:A:1104:CYS:O	1:A:1108:LEU:HD13	2.17	0.44
1:A:109:SER:CB	1:A:110:PRO:HD3	2.47	0.44
1:A:795:LEU:CD2	1:A:806:ILE:HB	2.47	0.44
1:A:477:VAL:CG2	1:A:478:PRO:CD	2.95	0.44
1:A:842:SER:N	1:A:845:LYS:O	2.48	0.44
1:A:499:ASP:CA	1:A:502:ILE:HG22	2.46	0.44
1:A:533:GLN:OE1	1:A:533:GLN:HA	2.17	0.44
1:A:808:GLU:HG3	1:A:809:ASN:OD1	2.18	0.44
1:A:990:VAL:CG1	1:A:1021:LEU:HD22	2.47	0.44
1:A:1495:ARG:NE	1:A:1508:GLY:HA2	2.32	0.44
1:A:643:SER:HG	1:A:821:THR:HG21	1.80	0.44
1:A:1361:GLY:O	1:A:1364:ASP:HB2	2.17	0.44
1:A:1422:CYS:SG	1:A:1426:GLY:HA2	2.57	0.44
1:A:46:LEU:HD22	1:A:141:PHE:CE2	2.52	0.44
1:A:75:THR:OG1	1:A:125:GLN:NE2	2.50	0.44
1:A:443:MET:HE2	1:A:594:PHE:CE2	2.52	0.44
1:A:451:VAL:HA	1:A:592:LEU:CD1	2.48	0.44
1:A:405:ARG:HH22	1:A:1178:ASP:CG	2.24	0.44
1:A:720:ILE:HG13	1:A:725:ASN:OD1	2.17	0.44
1:A:1259:ALA:O	1:A:1263:LEU:HG	2.17	0.44
1:A:68:THR:OG1	1:A:69:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:HG3	1:A:1262:ARG:HD2	2.00	0.44
1:A:1319:GLY:N	1:A:1479:THR:OG1	2.51	0.44
1:A:1121:LEU:HD11	1:A:1208:CYS:HB2	2.00	0.43
1:A:1145:VAL:HG12	1:A:1145:VAL:O	2.18	0.43
1:A:341:ALA:O	1:A:345:ILE:HG13	2.17	0.43
1:A:741:VAL:HG23	1:A:746:LEU:CD1	2.47	0.43
1:A:836:ASP:OD2	1:A:836:ASP:C	2.61	0.43
1:A:840:VAL:O	1:A:847:SER:HB3	2.17	0.43
1:A:981:PHE:CZ	1:A:1032:TYR:CE2	3.07	0.43
1:A:1467:ILE:O	1:A:1470:THR:OG1	2.30	0.43
1:A:761:ILE:CG2	1:A:761:ILE:O	2.67	0.43
1:A:6:PHE:CE2	1:A:105:VAL:HB	2.53	0.43
1:A:499:ASP:HA	1:A:502:ILE:CG2	2.48	0.43
1:A:508:ILE:CD1	1:A:524:PHE:HB3	2.48	0.43
1:A:1299:LEU:H	1:A:1309:LEU:CG	2.31	0.43
1:A:1381:GLY:HA3	1:A:1385:MET:HG2	2.00	0.43
1:A:15:PHE:HD1	1:A:32:CYS:SG	2.42	0.43
1:A:676:VAL:CB	1:A:839:ILE:HG13	2.48	0.43
1:A:741:VAL:CG2	1:A:746:LEU:HB2	2.48	0.43
1:A:1056:LEU:HD13	1:A:1056:LEU:HA	1.86	0.43
1:A:665:THR:O	1:A:665:THR:HG23	2.18	0.43
1:A:750:LEU:HA	1:A:753:LEU:CD2	2.49	0.43
1:A:774:GLN:CD	1:A:794:PRO:O	2.62	0.43
1:A:791:LEU:CD2	1:A:811:ILE:HD13	2.49	0.43
1:A:1410:PHE:O	1:A:1413:ALA:HB3	2.17	0.43
1:A:794:PRO:HD2	1:A:824:LEU:HD11	2.00	0.43
1:A:1122:GLY:O	1:A:1126:PHE:HB3	2.18	0.43
1:A:1486:ARG:O	1:A:1487:LEU:C	2.61	0.43
1:A:1496:VAL:O	1:A:1497:ILE:HG13	2.18	0.43
1:A:632:ARG:HH22	1:A:708:VAL:HG11	1.83	0.43
1:A:658:PRO:HA	1:A:659:PRO:HD2	1.91	0.43
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.82	0.43
1:A:1336:THR:O	1:A:1337:LEU:C	2.62	0.43
1:A:56:TYR:CD1	1:A:57:LEU:HD12	2.54	0.42
1:A:580:GLN:O	1:A:584:VAL:HB	2.19	0.42
1:A:582:ALA:C	1:A:584:VAL:H	2.26	0.42
1:A:1203:GLU:OE2	1:A:1240:THR:O	2.37	0.42
1:A:1240:THR:HG23	1:A:1241:THR:N	2.34	0.42
1:A:1362:LEU:HD22	1:A:1366:ARG:NE	2.34	0.42
1:A:1376:PRO:HB2	1:A:1434:ARG:CB	2.49	0.42
1:A:244:LEU:HD11	1:A:1185:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:O	1:A:426:LEU:HD13	2.19	0.42
1:A:436:ASP:O	1:A:439:THR:HG22	2.19	0.42
1:A:515:LEU:HD21	1:A:524:PHE:CD2	2.54	0.42
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.79	0.42
1:A:1372:ILE:O	1:A:1372:ILE:HG22	2.19	0.42
1:A:67:MET:HE2	1:A:67:MET:HB2	1.91	0.42
1:A:684:LYS:C	1:A:686:SER:H	2.28	0.42
1:A:846:ILE:CD1	1:A:849:MET:SD	3.06	0.42
1:A:965:TYR:CZ	1:A:969:ILE:HD11	2.52	0.42
1:A:1275:TRP:CG	1:A:1363:HIS:CD2	3.08	0.42
1:A:339:MET:HE1	1:A:450:GLN:OE1	2.20	0.42
1:A:753:LEU:HD11	1:A:756:GLY:CA	2.49	0.42
1:A:789:TYR:HB3	1:A:791:LEU:HD11	2.01	0.42
1:A:479:LEU:O	1:A:483:MET:HG2	2.20	0.42
1:A:558:PHE:CE2	1:A:1022:GLY:HA3	2.51	0.42
1:A:657:ASP:HB3	1:A:658:PRO:CD	2.42	0.42
1:A:1079:LEU:HD12	1:A:1079:LEU:HA	1.84	0.42
1:A:1499:LEU:HA	1:A:1505:GLN:CB	2.48	0.42
1:A:81:LEU:HA	1:A:84:VAL:HG12	2.02	0.42
1:A:710:TYR:CE2	1:A:712:PRO:HB3	2.55	0.42
1:A:798:VAL:HG11	1:A:802:VAL:HG12	2.02	0.42
1:A:1088:GLN:N	1:A:1088:GLN:OE1	2.53	0.42
1:A:1108:LEU:O	1:A:1112:PRO:HA	2.19	0.42
1:A:162:LYS:HE3	1:A:163:GLU:OE1	2.20	0.42
1:A:654:ALA:CB	1:A:657:ASP:OD1	2.68	0.42
1:A:664:ILE:CG2	1:A:666:PHE:CE1	3.03	0.42
1:A:49:CYS:O	1:A:53:TYR:HB2	2.20	0.42
1:A:493:ALA:HB1	1:A:496:LYS:HZ1	1.84	0.42
1:A:19:ASN:CB	2:A:1601:NAG:N2	2.83	0.42
1:A:13:ASP:OD1	1:A:13:ASP:O	2.38	0.41
1:A:364:TYR:O	1:A:367:THR:HG22	2.20	0.41
1:A:434:PHE:HZ	1:A:613:LEU:CB	2.33	0.41
1:A:644:ILE:HD12	1:A:668:VAL:HG21	2.02	0.41
1:A:731:GLN:O	1:A:731:GLN:OE1	2.38	0.41
1:A:994:TRP:CZ2	1:A:1014:ARG:HD3	2.54	0.41
1:A:1322:VAL:CA	1:A:1493:TYR:HD2	2.33	0.41
1:A:1495:ARG:HA	1:A:1510:PRO:HD3	2.02	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.84	0.41
1:A:165:ALA:O	1:A:166:ARG:NH2	2.52	0.41
1:A:250:SER:OG	1:A:1182:ASP:OD1	2.21	0.41
1:A:327:MET:HA	1:A:327:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:HG22	1:A:698:VAL:HG23	2.02	0.41
1:A:722:LEU:HD11	1:A:776:VAL:HG22	2.00	0.41
1:A:733:GLN:O	1:A:734:GLU:C	2.63	0.41
1:A:832:LEU:N	1:A:833:PRO:CD	2.83	0.41
1:A:995:LEU:O	1:A:995:LEU:HD12	2.20	0.41
1:A:1296:ASP:HA	1:A:1311:HIS:O	2.19	0.41
1:A:1497:ILE:HD12	1:A:1497:ILE:N	2.35	0.41
1:A:6:PHE:O	1:A:103:ALA:HB1	2.20	0.41
1:A:81:LEU:HD23	1:A:181:LEU:CD2	2.50	0.41
1:A:127:GLU:CB	1:A:132:VAL:CG1	2.98	0.41
1:A:224:ILE:HG12	1:A:224:ILE:O	2.20	0.41
1:A:722:LEU:HD13	1:A:761:ILE:HD11	2.02	0.41
1:A:746:LEU:HD23	1:A:749:ASP:OD2	2.20	0.41
1:A:958:LYS:C	1:A:960:SER:N	2.79	0.41
1:A:962:TYR:HE1	1:A:1253:MET:HE3	1.84	0.41
1:A:1165:ARG:HG3	1:A:1170:GLN:NE2	2.34	0.41
1:A:1341:ARG:NH1	1:A:1357:ILE:O	2.53	0.41
1:A:1360:ILE:CG1	1:A:1361:GLY:N	2.83	0.41
1:A:1490:ILE:O	1:A:1493:TYR:HB2	2.20	0.41
1:A:330:LEU:C	1:A:330:LEU:HD23	2.45	0.41
1:A:761:ILE:HG22	1:A:765:GLY:H	1.83	0.41
1:A:1111:THR:O	1:A:1111:THR:OG1	2.35	0.41
1:A:1494:THR:OG1	1:A:1495:ARG:N	2.52	0.41
1:A:473:MET:CG	1:A:596:LEU:HD11	2.50	0.41
1:A:832:LEU:HD12	1:A:832:LEU:N	2.34	0.41
1:A:1013:VAL:O	1:A:1016:SER:OG	2.33	0.41
1:A:1433:GLN:C	1:A:1437:VAL:HG23	2.42	0.41
1:A:346:LEU:HD13	1:A:1233:VAL:CG1	2.50	0.41
1:A:444:ILE:CD1	1:A:606:ILE:HD12	2.45	0.41
1:A:524:PHE:N	1:A:524:PHE:CD1	2.88	0.41
1:A:583:PHE:HE1	1:A:1231:LEU:HD12	1.86	0.41
1:A:738:LYS:C	1:A:741:VAL:HG12	2.46	0.41
1:A:1277:ILE:O	1:A:1281:ALA:HA	2.19	0.41
1:A:1347:GLU:OE1	1:A:1347:GLU:HA	2.21	0.41
1:A:96:ARG:HH11	1:A:96:ARG:HG2	1.86	0.41
1:A:142:TRP:CE3	1:A:142:TRP:HA	2.56	0.41
1:A:734:GLU:OE1	1:A:734:GLU:N	2.51	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.85	0.41
1:A:613:LEU:C	1:A:613:LEU:HD23	2.45	0.41
1:A:753:LEU:HD11	1:A:756:GLY:HA2	2.03	0.41
1:A:1117:ILE:CG2	1:A:1212:PHE:CD2	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:VAL:CG2	1:A:1197:TRP:CZ3	3.03	0.41
1:A:71:ASN:OD1	1:A:72:LYS:N	2.54	0.41
1:A:101:LEU:C	1:A:102:LEU:HD12	2.45	0.41
1:A:544:TYR:CD1	1:A:1034:MET:SD	3.14	0.41
1:A:799:ASP:OD1	1:A:799:ASP:C	2.63	0.41
1:A:866:LEU:HD12	1:A:870:ALA:HB2	2.02	0.41
1:A:1147:ARG:HG3	1:A:1184:ASN:HD21	1.86	0.41
1:A:1352:ILE:O	1:A:1355:ILE:HG13	2.21	0.41
1:A:1475:PHE:O	1:A:1478:CYS:N	2.42	0.41
1:A:40:TRP:O	1:A:44:SER:HB3	2.21	0.41
1:A:409:VAL:HG12	1:A:409:VAL:O	2.21	0.41
1:A:722:LEU:HD12	1:A:761:ILE:HD11	2.02	0.41
1:A:493:ALA:HA	1:A:496:LYS:CE	2.51	0.40
1:A:540:LYS:HA	1:A:1041:ILE:HD11	2.03	0.40
1:A:6:PHE:CD2	1:A:105:VAL:HB	2.57	0.40
1:A:208:CYS:HA	1:A:209:PRO:HD3	1.90	0.40
1:A:726:ILE:HD11	1:A:746:LEU:CD1	2.50	0.40
1:A:769:SER:O	1:A:770:GLY:C	2.64	0.40
1:A:810:VAL:HG23	1:A:811:ILE:HG12	2.02	0.40
1:A:832:LEU:CD1	1:A:832:LEU:H	2.32	0.40
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.86	0.40
1:A:664:ILE:CG2	1:A:666:PHE:CD1	3.04	0.40
1:A:673:LEU:HB2	1:A:822:ARG:CZ	2.51	0.40
1:A:739:ALA:HA	1:A:742:GLU:HG3	2.04	0.40
1:A:1148:SER:OG	1:A:1149:PRO:CD	2.67	0.40
1:A:1169:GLU:O	1:A:1173:PHE:HD1	2.03	0.40
1:A:1290:GLY:O	1:A:1318:GLY:HA2	2.21	0.40
1:A:1499:LEU:HA	1:A:1505:GLN:N	2.36	0.40
1:A:50:PHE:HB3	1:A:51:PRO:HD3	2.02	0.40
1:A:125:GLN:OE1	1:A:125:GLN:HA	2.21	0.40
1:A:512:ILE:HG12	1:A:1063:PHE:CD2	2.56	0.40
1:A:588:LEU:O	1:A:592:LEU:HB2	2.22	0.40
1:A:646:VAL:O	1:A:665:THR:HA	2.22	0.40
1:A:668:VAL:O	1:A:668:VAL:HG23	2.20	0.40
1:A:1322:VAL:HG22	1:A:1494:THR:OG1	2.21	0.40
1:A:1372:ILE:O	1:A:1373:PRO:C	2.64	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	1394/1530 (91%)	1280 (92%)	114 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1053/1336 (79%)	1053 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	377	GLN
1	A	412	ASN
1	A	442	ASN
1	A	491	GLN
1	A	590	ASN
1	A	631	GLN
1	A	656	ASN
1	A	719	ASN
1	A	992	ASN
1	A	1053	HIS

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Mol	Chain	Res	Type
1	A	1170	GLN
1	A	1184	ASN
1	A	1238	GLN
1	A	1244	ASN
1	A	1276	GLN
1	A	1363	HIS
1	A	1420	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1601	1	14,14,15	2.24	4 (28%)	17,19,21	1.43	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1601	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	NAG	O5-C1	5.67	1.52	1.43
2	A	1601	NAG	C7-N2	3.91	1.47	1.34
2	A	1601	NAG	C2-N2	2.90	1.51	1.46
2	A	1601	NAG	O7-C7	-2.15	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	NAG	C1-O5-C5	3.93	117.51	112.19
2	A	1601	NAG	C8-C7-N2	2.28	119.96	116.10
2	A	1601	NAG	C2-N2-C7	-2.12	119.88	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	NAG	2	0

## 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.

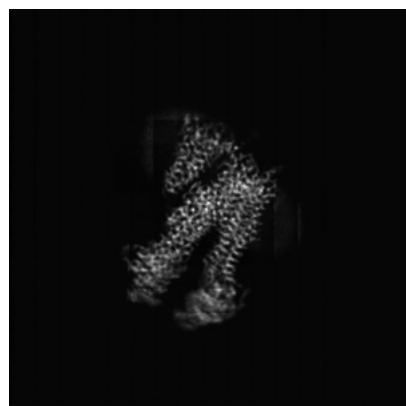
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61270. These allow visual inspection of the internal detail of the map and identification of artifacts.

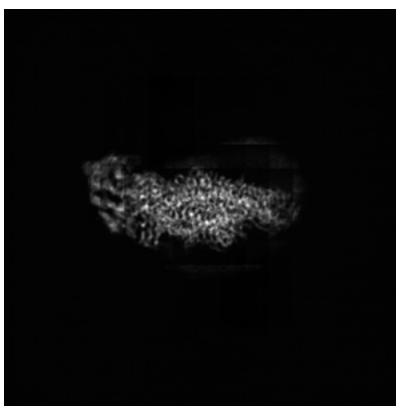
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

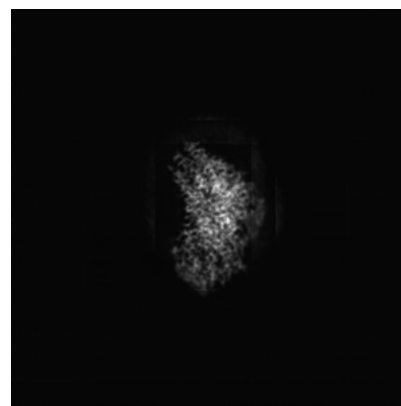
#### 6.1.1 Primary map



X

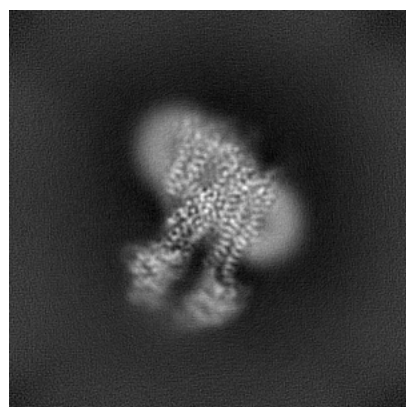


Y

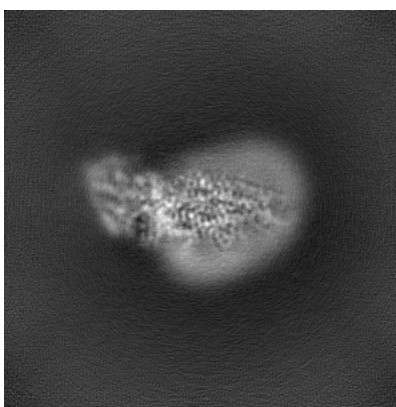


Z

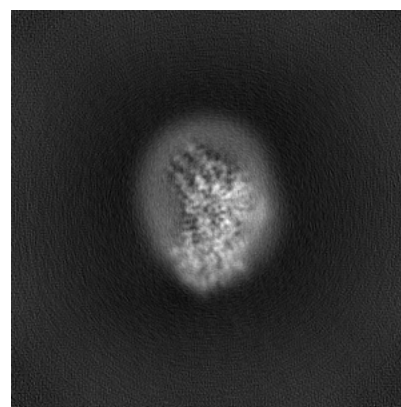
#### 6.1.2 Raw map



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: 160

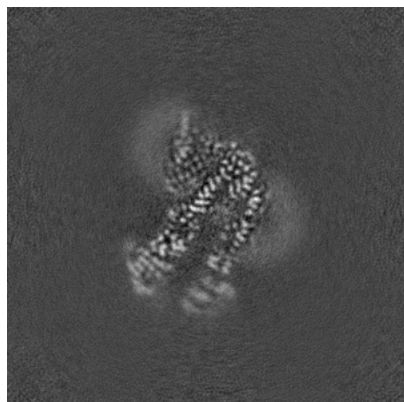


Y Index: 160

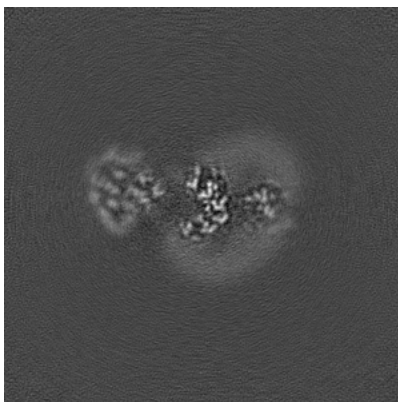


Z Index: 160

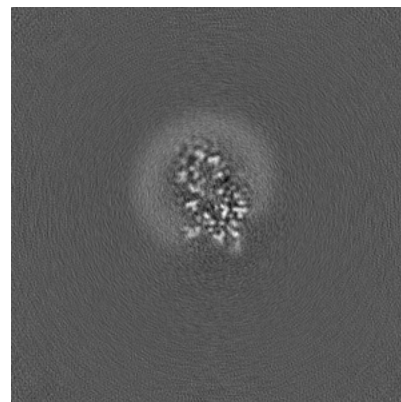
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 169

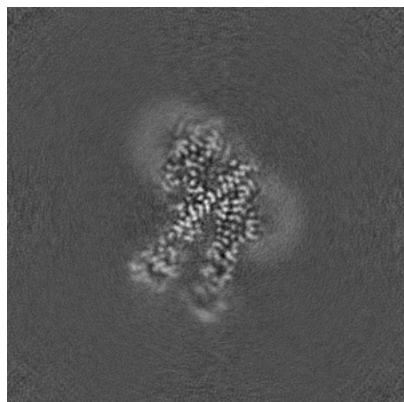


Y Index: 178

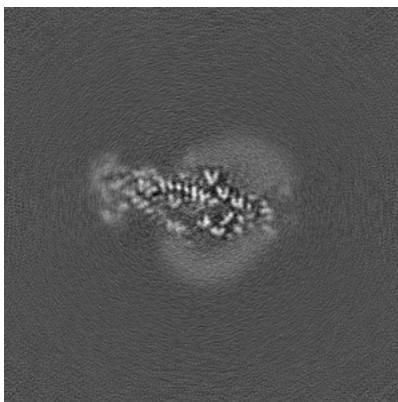


Z Index: 164

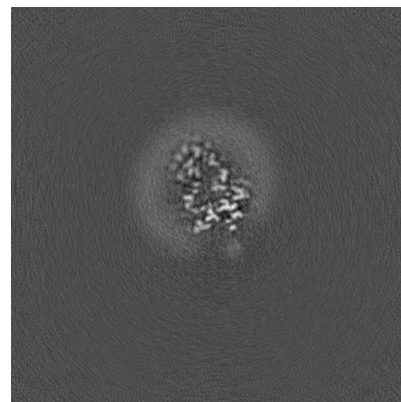
### 6.3.2 Raw map



X Index: 169



Y Index: 173

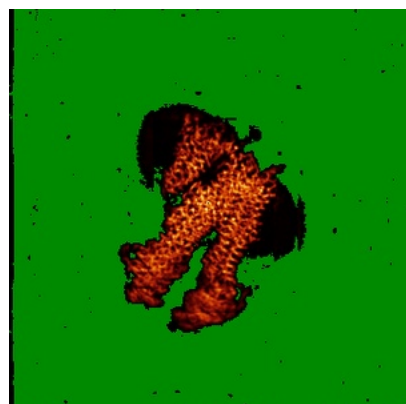


Z Index: 164

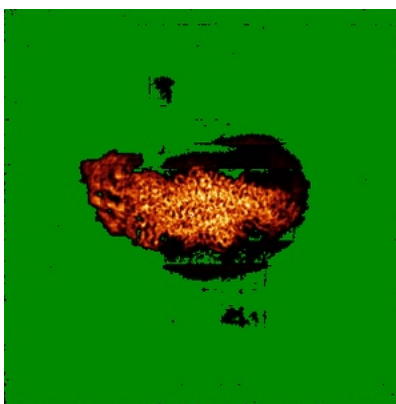
The images above show the largest variance slices of the map in three orthogonal directions.

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

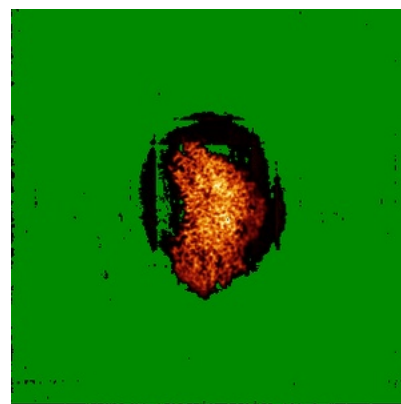
### 6.4.1 Primary map



X

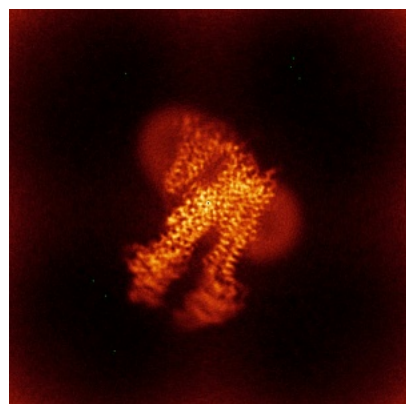


Y

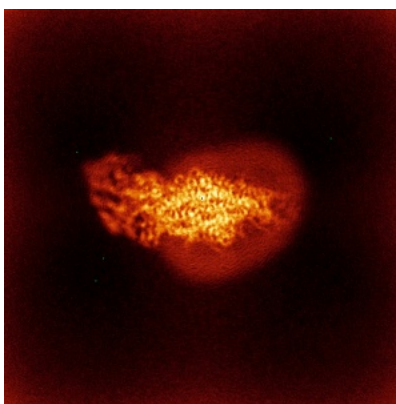


Z

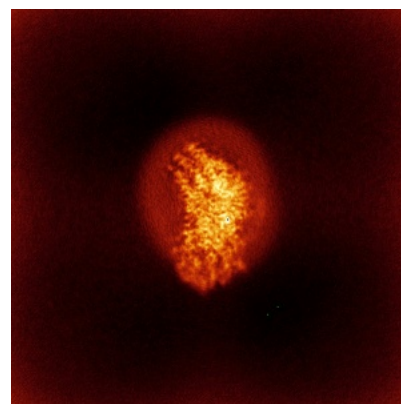
### 6.4.2 Raw map



X



Y

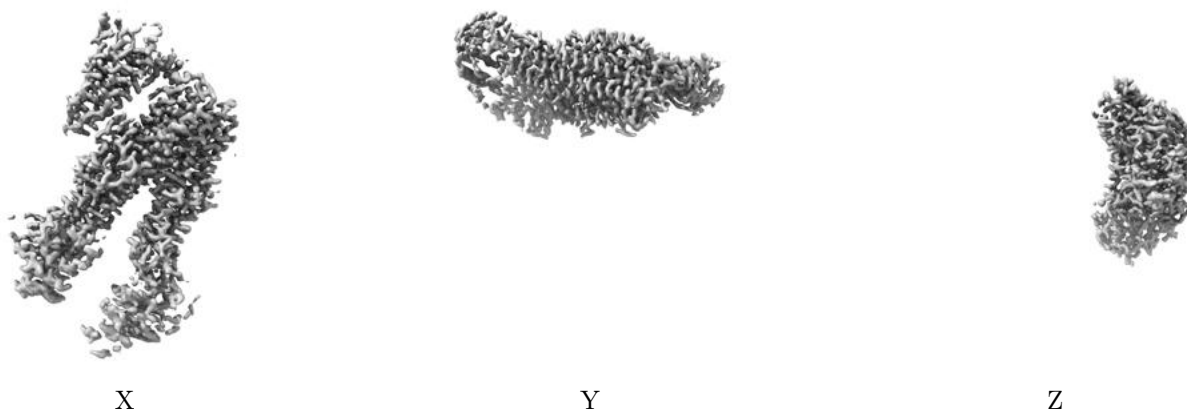


Z

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.

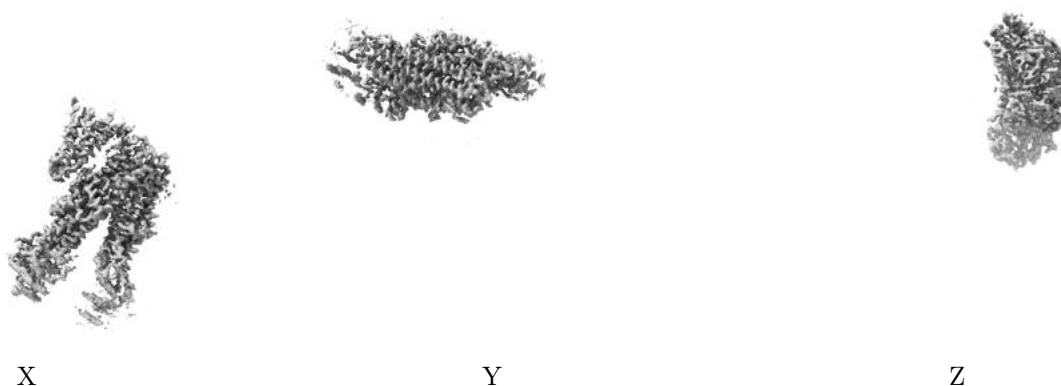
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

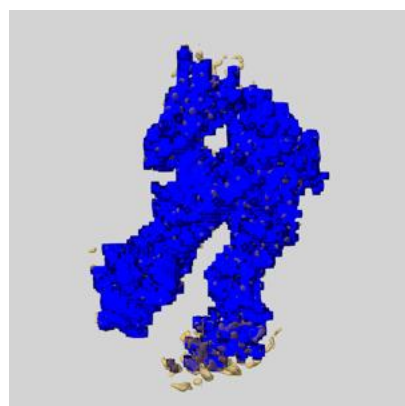
## 6.6 Mask visualisation [i](#)

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

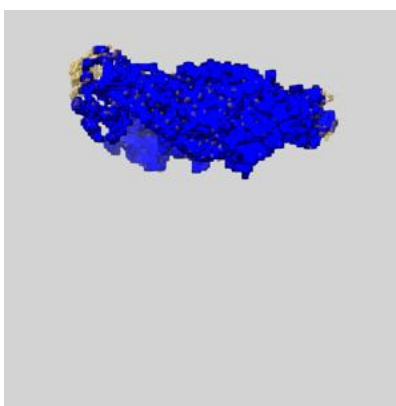
A mask typically either:

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

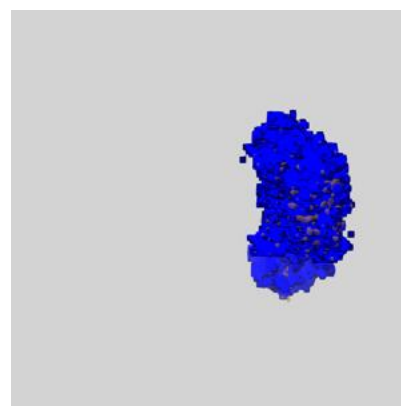
### 6.6.1 emd\_61270\_msk\_1.map [i](#)



X



Y

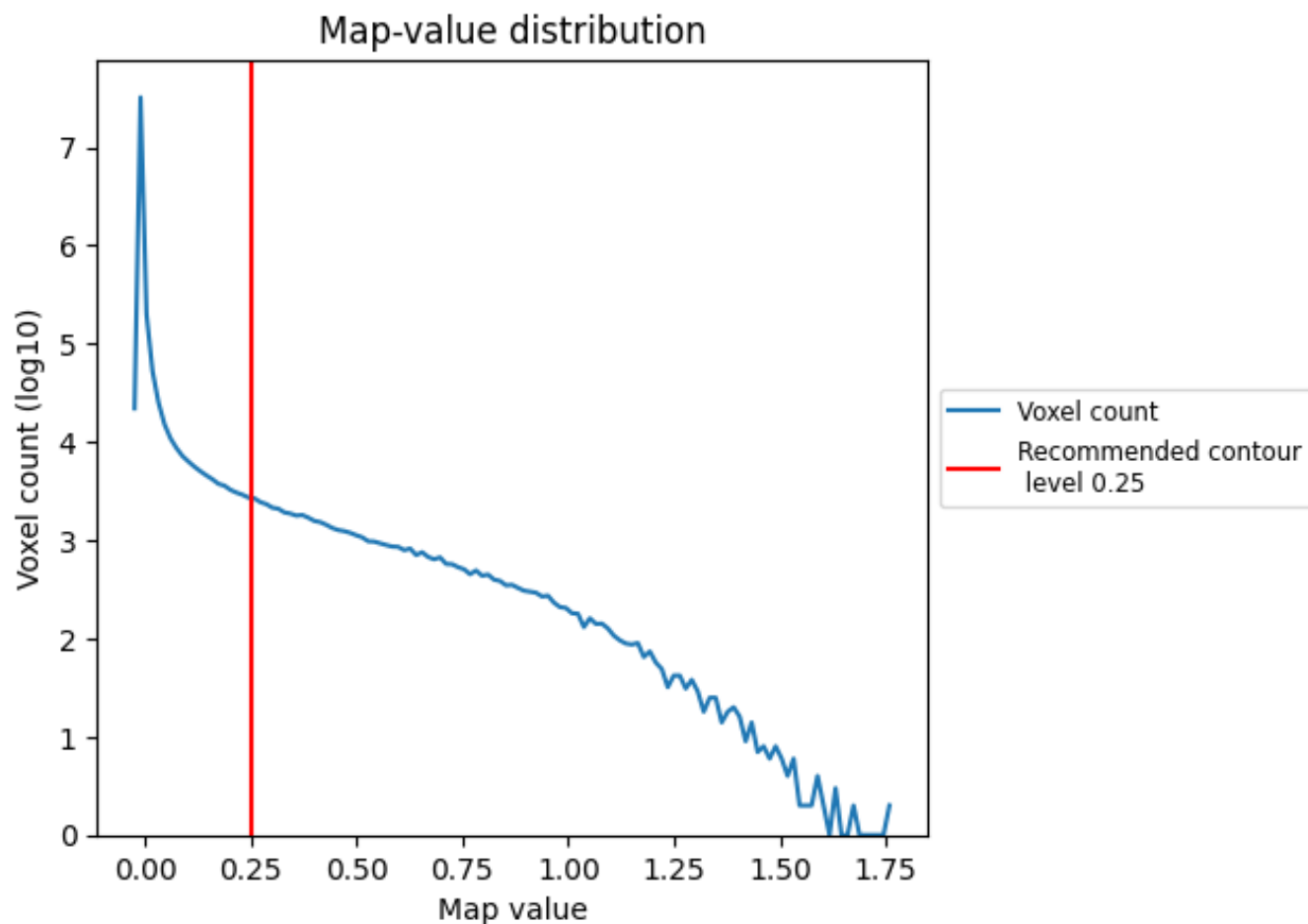


Z

## 7 Map analysis [i](#)

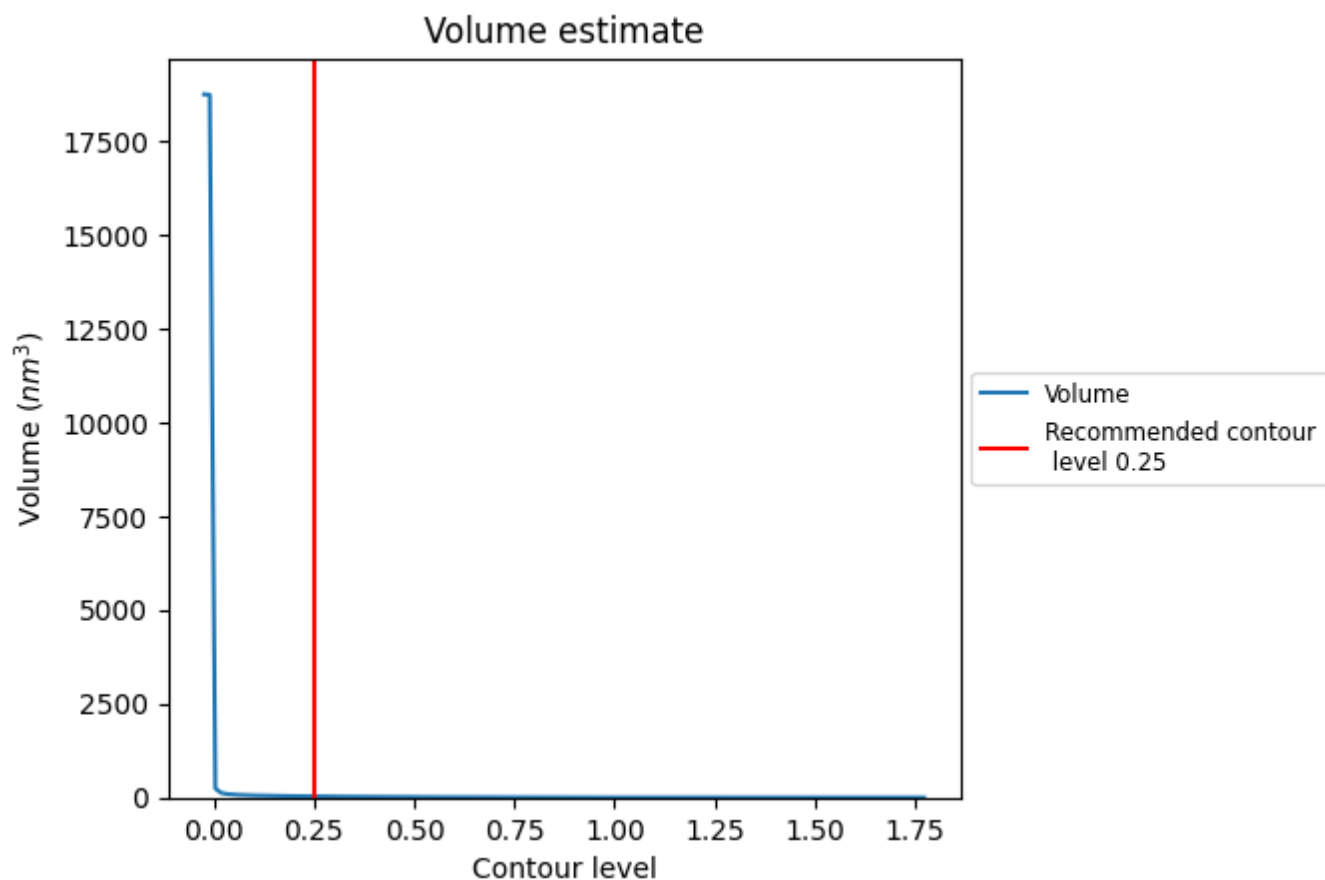
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

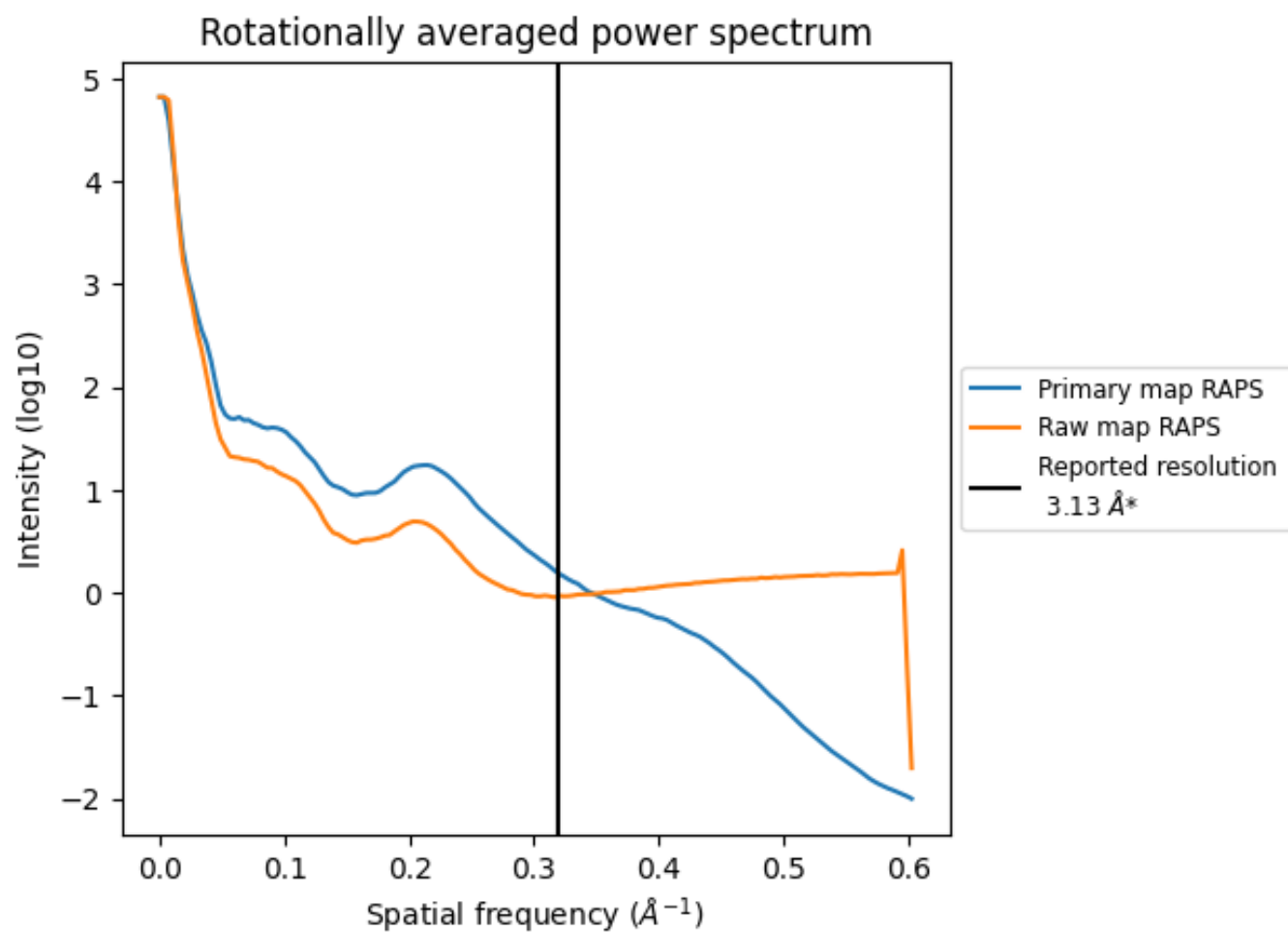
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31  $\text{nm}^3$ ; this corresponds to an approximate mass of 28 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 ⓘ

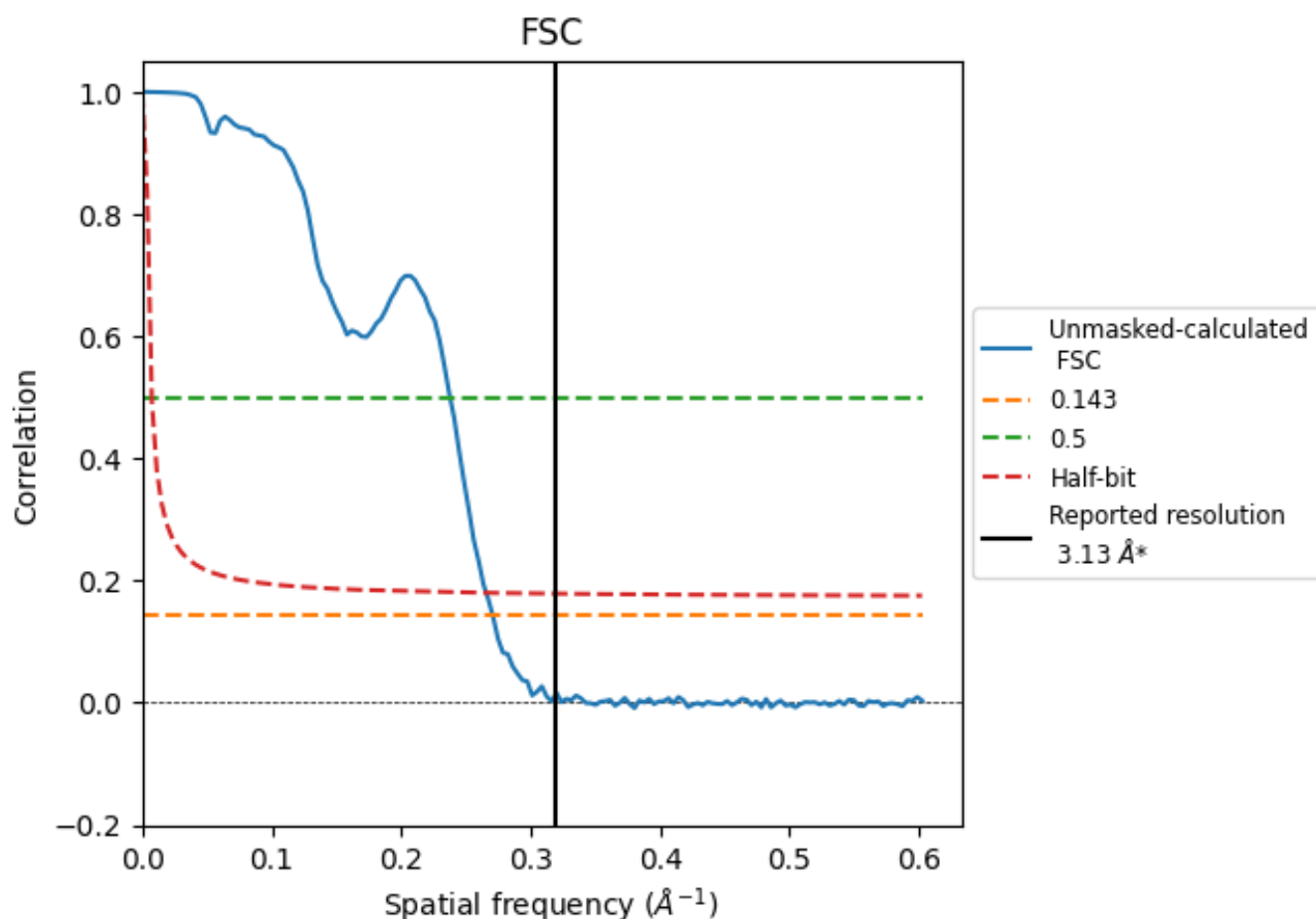


\*Reported resolution corresponds to spatial frequency of 0.319 Å<sup>-1</sup>

## 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  $0.319 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

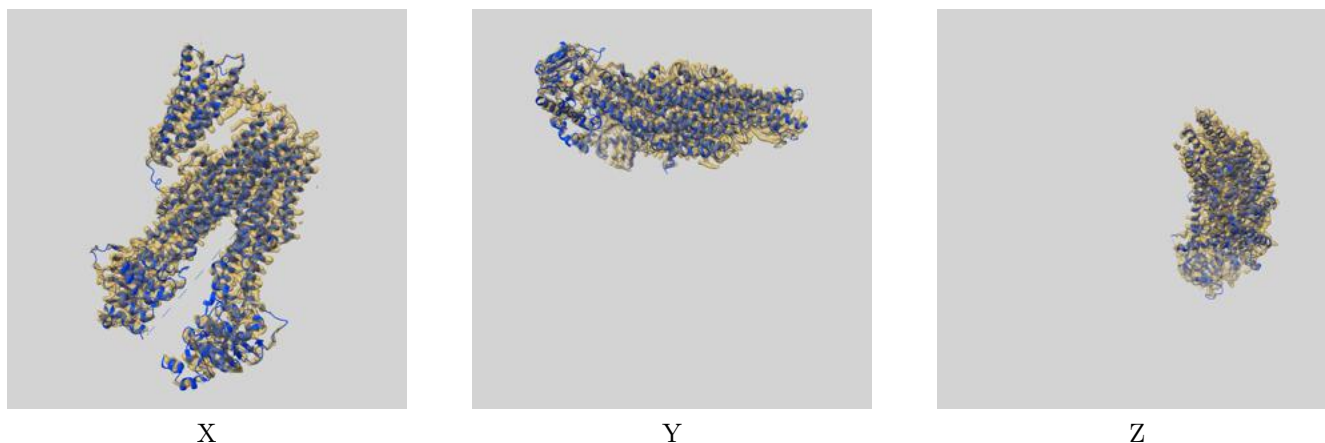
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.21	3.76

\*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 3.69 differs from the reported value 3.13 by more than 10 %

## 9 Map-model fit [i](#)

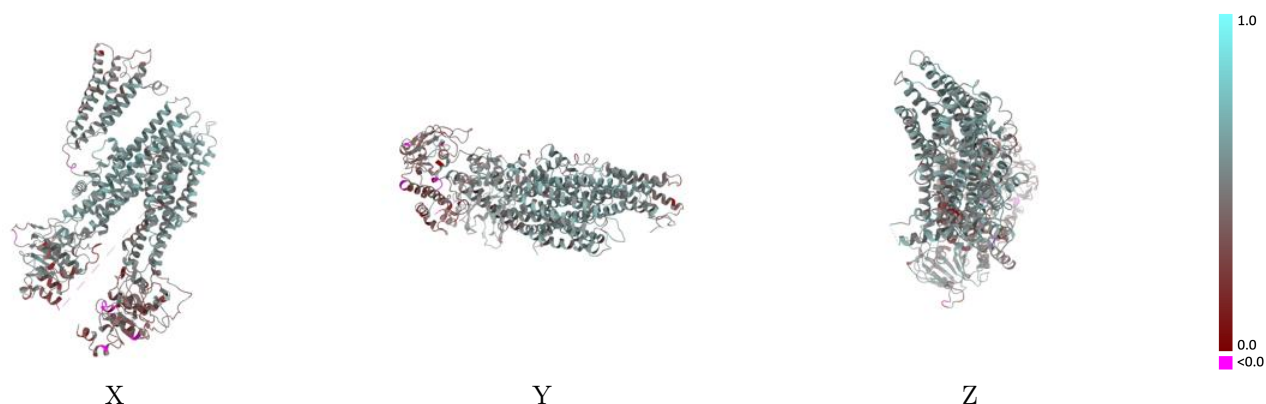
This section contains information regarding the fit between EMDB map EMD-61270 and PDB model 9J9F. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

### 9.1 Map-model overlay [i](#)



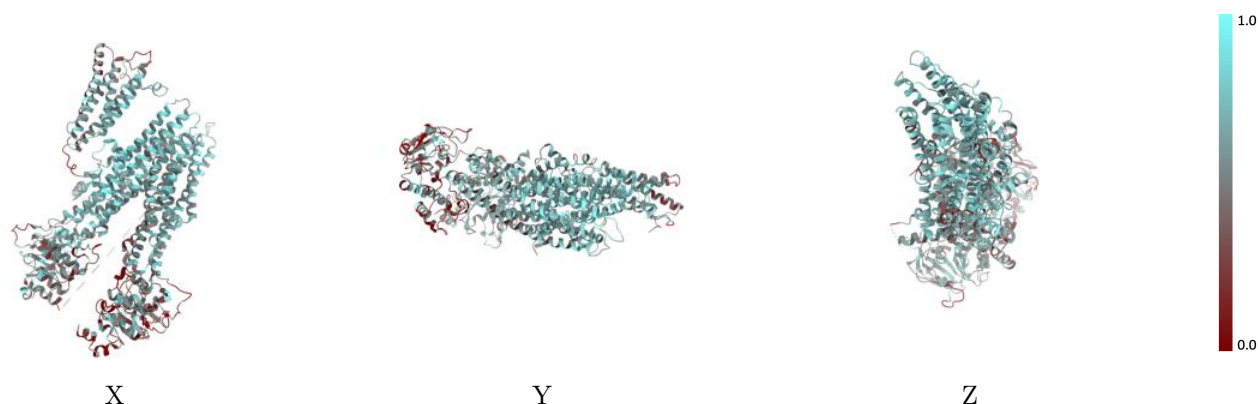
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



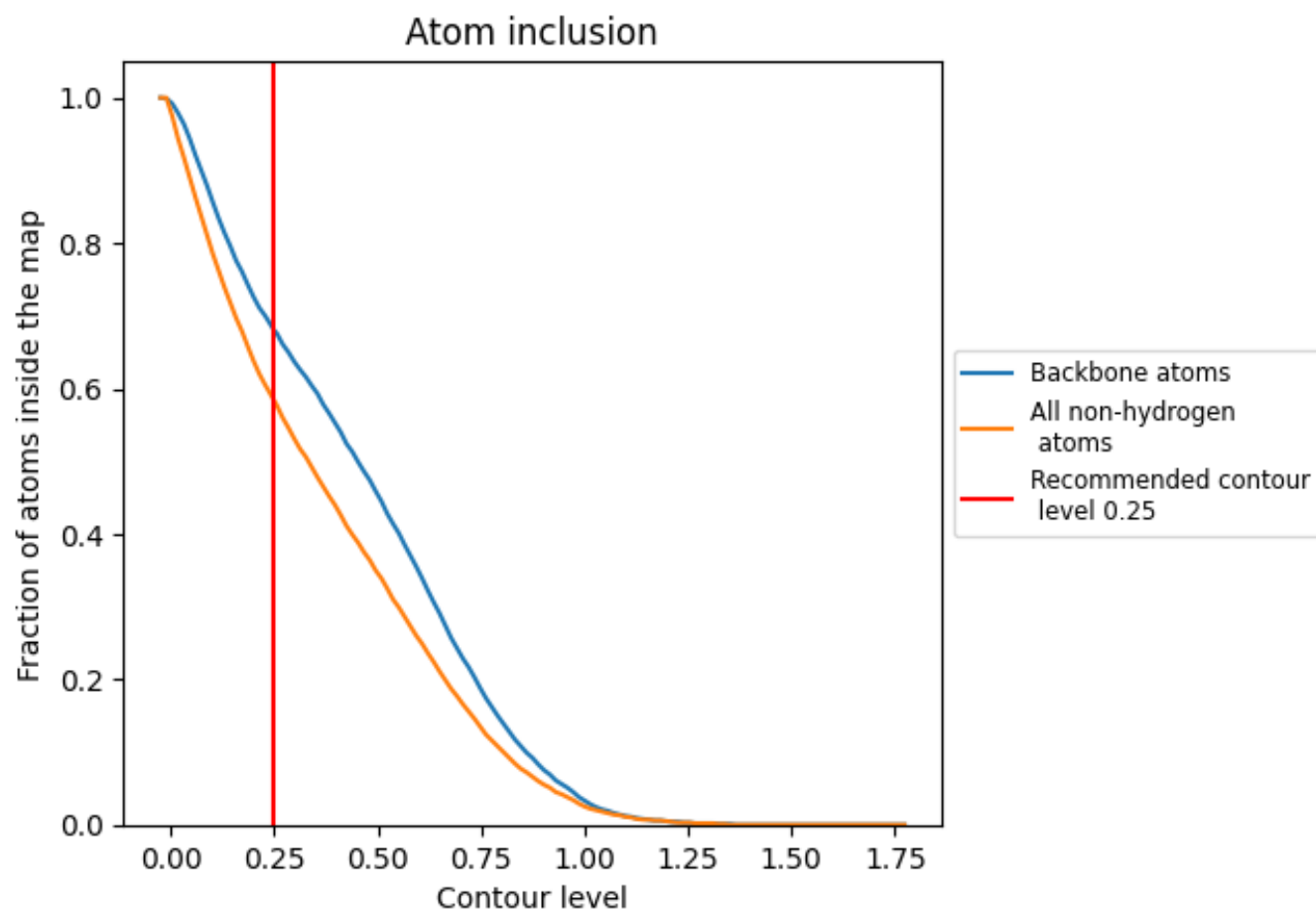
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 58% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5830	<div></div> 0.4930
A	<div></div> 0.5830	<div></div> 0.4930

