



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:29 PM UTC

PDB ID : 8V0G / pdb_00008v0g
EMDB ID : EMD-42854
Title : plasmodium falciparum Niemann-Pick type C1-related protein form I
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2023-11-17
Resolution : 3.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

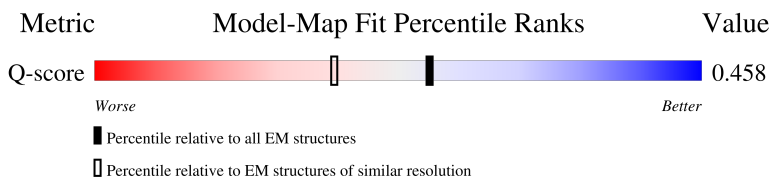
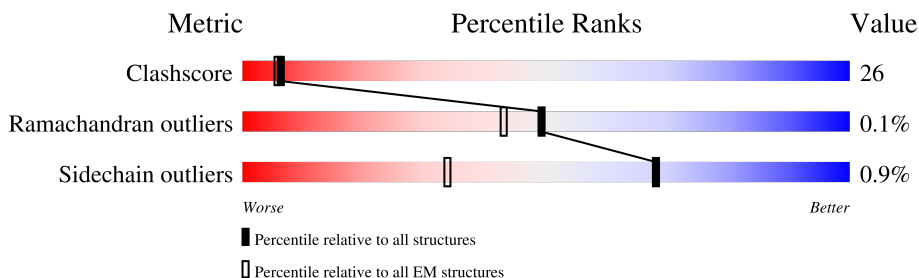
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	1470	

2 Entry composition [i](#)

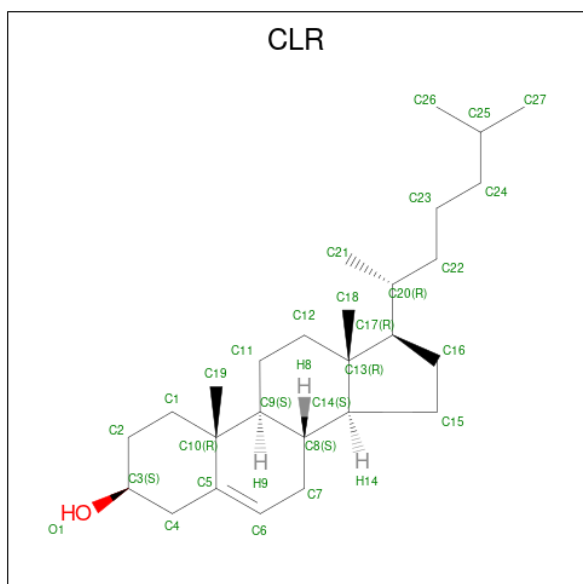
There are 3 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Niemann-Pick type C1-related protein.

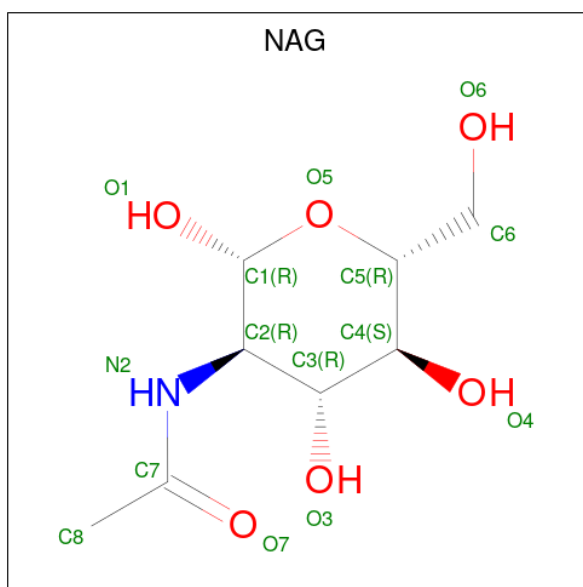
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	985	8050	5285	1266	1454	45	0	0

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	28	27	1	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

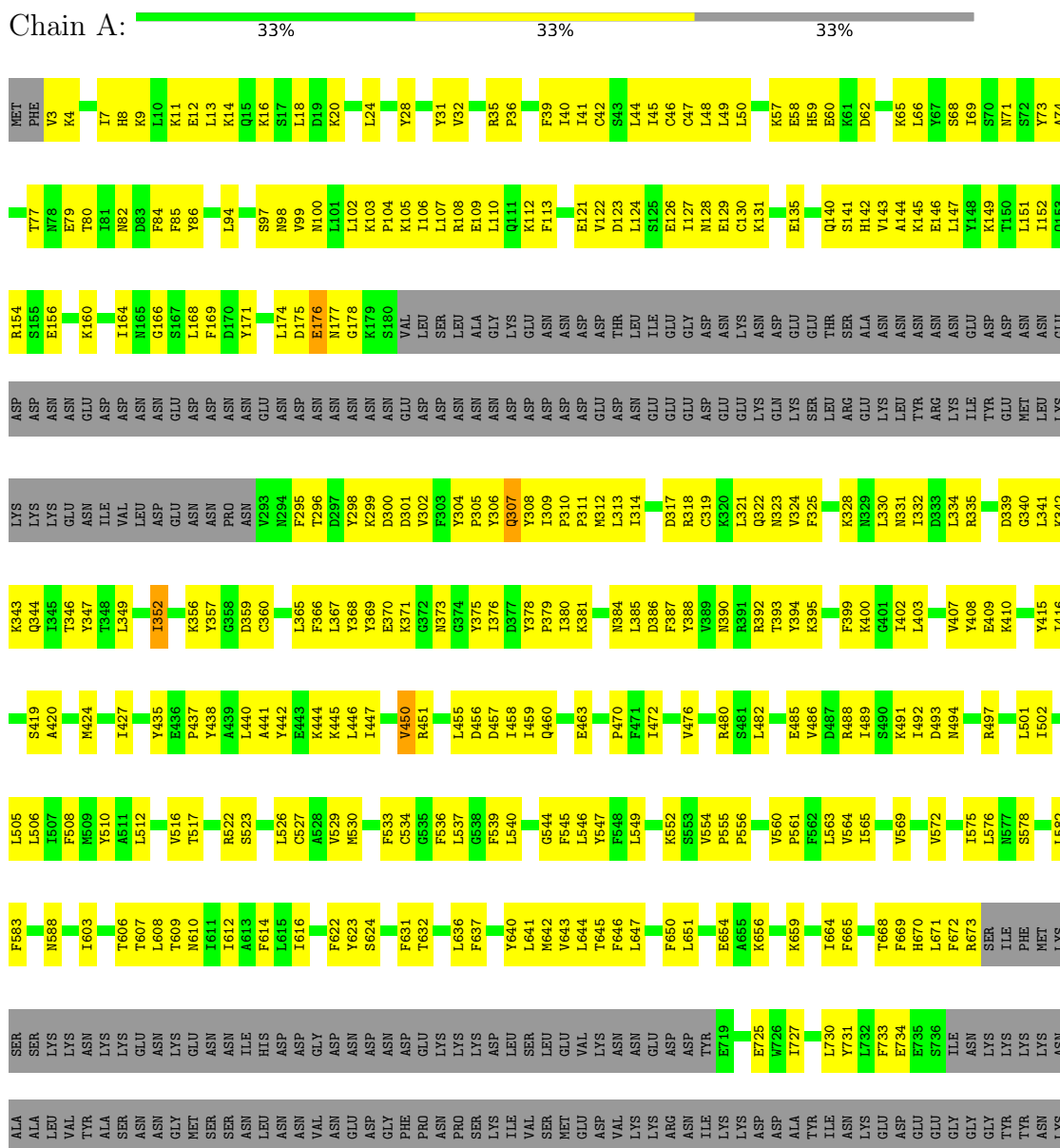


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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: Niemann-Pick type C1-related protein



I1452	M1367	K1284	S1200	D1128	PHE	ASP	SER	ASN	ASP
T1453	I1368	Q1285	Q1201	F1129	TTR	ILE	SER	ASP	ASP
	I1369	E1286	E1202		K1046	ILE	TYR	ASP	ASN
S1456	S1370		F1203	F1132	Y1047	ASN	ASN	LYS	LYS
M1457	M1371	L1289	V1204		I1048	SER	ASP	ASP	LYS
F1458	V1372	H1292	T1205	V1135	Y1049	ASN	LEU	GLY	LYS
L1459	I1373	H1293	S1206		E1050	ASN	GLN	ALA	ASP
P1460		V1207		F1138	E1051	LYS	SER	ILE	ASP
	L1376			D1139	P1052	ASN	SER	ILE	ILE
F1466		V1294	G1210	K1140	K1053	ASN	SER	ASN	LEU
G1467	G1379	Q1295	F1211	H1141	K1054	ILE	SER	ASN	GLY
P1468	M1296	M1296	F1212	F1142	N1055	LEU	LEU	ASN	LYS
L1469		F1213	F1212	I1143	I1056	SER	PRO	ARG	LYS
H1470	I1382	L1301	F1214		G1057	ASN	PRO	GLN	LYS
	D1383			Y1146	K1058	SER	SER	LYS	LYS
	H1384	I1304		R1147	Y1059	ASN	SER	LYS	LYS
	T1385	F1305	N1218	G1148	F1060	GLU	ASP	ASN	ASN
				L1149	R1061	ASN	GLU	ASN	ASN
V1389	V1308	T1309	L1222	E1150	S1062	ASN	VAL	TYR	ASN
Q1390	D1309			K1151	L1063	ASN	LEU	LYS	VAL
A1391		N1226	N1227	ASN	V1064	SER	ASN	THR	THR
F1392	I1312	Q1228	Q1228	THR		ASN	LYS	GLU	THR
S1393	I1313	E1229	E1229	LYS	Y1067	ASN	THR	LYS	VAL
H1394	E1314	F1230	F1230	GLU	Y1068	ASN	THR	LYS	VAL
S1395	V1315	Y1231	Y1231	ALA	V1069	ASN	MET	LYS	SER
M1396	T1316	E1232	E1232	ALA	P1070	LYS	VAL	LYS	LYS
G1397	L1317	I1233	I1233	SER	F1071	PHE	TYR	GLY	GLY
R1398	I1318	F1234	F1234	ASN	L1072	ASN	ASN	ILE	GLY
T1399				PHE	F1076	ASN	GLU	ILE	ASN
R1400	I1322	K1240	K1240	LEU	G1077	ASN	THR	LEU	ASN
D1401	T1323	D1241	D1241	TYR	K1078	ASN	ASP	GLU	GLU
E1402	I1324	F1242	F1242	SER	T1079	GLU	LYS	LEU	LEU
K1403				ASP	I1080	LEU	ASP	VAL	VAL
M1404	I1327	L1246	L1246	THR		ALA	ASP	PHE	TYR
K1405		F1247	F1247	ASP	I1083	THR	LYS	ASN	TYR
	T1331	K1248	K1248	ARG	M1084	LYS	ASP	GLU	GLU
L1410	A1332	N1249	N1249	G1169	F1086	ASP	ILE	THR	ASN
M1411	Y1333	L1254	L1254	I1170	I1087	THR	ILE	THR	LEU
I1412	I1334	N1255	N1255	M1171	I1088	GLN	ILE	ASP	ASP
G1413	I1335	G1256	G1256	N1172	I1089	SER	SER	GLY	GLY
P1414	K1336			S1173		PHE	PRO	LYS	LYS
		W1261	W1261	P1174		ILE	ASN	THR	THR
H1417	Y1339			K1175	Y1094	ASN	LYS	ASN	ASN
S1418	S1340			I1176		GLY	ASN	ASP	ASP
G1419	G1341	Y1265	Y1265	M1177	L1098	HIS	VAL	LYS	LYS
	V1342	F1266	F1266	K1178		ASN	LYS	LEU	TYR
W1423	I1343	Q1267	Q1267		K1104	LYS	ASP	LEU	TYR
	I1344					ASN	ILE	ASP	MET
I1426				M1184	K1107	ILE	LYS	ARG	ASN
S1427	I1347	V1270	V1270	T1185		TYR	LYS	GLY	ASN
		D1271	D1271	N1186		LEU	ASP	VAL	ILE
F1430	L1350	D1272	D1272	L1187	D1112	LEU	SER	VAL	LYS
	I1351			Q1188	S1113	LEU	MET	ILE	LYS
D1435	D1352	I1275	I1275	E1189		SER	ILE	SER	SER
		S1276	S1276		R1116	SER	LYS	LYS	LYS
V1438	I1355	S1277	S1277	I1192		HIS	ASP	ASP	LYS
	F1356	K1278	K1278	M1193	T1120	ASN	ASP	GLY	LEU
F1441		W1279	W1279	M1194		ASN	THR	TYR	LYS
Q1442	M1359	L1280	L1280	H1195	F1126	ALA	ASP	TYR	TYR
		K1281	K1281		P1127	LEU	ASP		ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63097	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 ($e^-/\text{\AA}^2$)	35.86	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.535	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.48	0/8239	0.68	1/11120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLU	N-CA-C	-5.17	105.77	111.71

There are no chirality outliers.

There are no planarity outliers.

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	8050	0	8078	417	0
2	A	28	0	46	7	0
3	A	28	0	26	1	0
All	All	8106	0	8150	418	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 26.

All (418) 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:530:MET:HB3	1:A:646:PHE:HE1	1.22	1.05
1:A:1400:ARG:HD3	1:A:1467:GLY:H	1.34	0.92
1:A:1177:ASN:HD21	1:A:1295:GLN:H	1.15	0.91
1:A:80:THR:HA	1:A:1147:ARG:HH21	1.36	0.91
1:A:517:THR:HG22	1:A:523:SER:HB3	1.57	0.85
1:A:530:MET:HB3	1:A:646:PHE:CE1	2.10	0.82
1:A:322:GLN:HB2	1:A:331:ASN:HA	1.60	0.82
1:A:312:MET:HG3	1:A:313:LEU:HD12	1.64	0.80
1:A:1128:ASP:HB3	1:A:1205:THR:HG21	1.62	0.80
1:A:609:THR:HG21	1:A:1382:ILE:HG21	1.63	0.79
1:A:69:ILE:HG13	1:A:1308:THR:HG22	1.64	0.78
1:A:313:LEU:HD11	1:A:1149:LEU:HD21	1.66	0.78
1:A:140:GLN:HB3	1:A:145:LYS:HD3	1.66	0.75
1:A:1055:ASN:HB2	1:A:1058:LYS:HB2	1.72	0.72
1:A:536:PHE:CE2	1:A:540:LEU:HD11	2.24	0.72
1:A:640:TYR:CE2	1:A:644:LEU:HD11	2.25	0.71
1:A:637:PHE:CE2	1:A:641:LEU:HD11	2.25	0.71
1:A:730:LEU:HD13	1:A:1049:TYR:HB3	1.73	0.71
1:A:328:LYS:HB3	1:A:330:LEU:HG	1.74	0.70
1:A:637:PHE:CZ	1:A:641:LEU:HD11	2.26	0.70
1:A:108:ARG:HG2	1:A:376:ILE:HG21	1.72	0.70
1:A:1052:PRO:HD2	1:A:1055:ASN:HD21	1.56	0.70
1:A:1173:SER:HB3	1:A:1176:ILE:HG12	1.73	0.69
1:A:556:PRO:HG2	1:A:624:SER:HB2	1.73	0.69
1:A:168:LEU:HD21	3:A:1502:NAG:H62	1.73	0.69
1:A:1402:GLU:O	1:A:1405:LYS:HG2	1.92	0.69
1:A:727:ILE:HG21	1:A:1410:LEU:HD11	1.76	0.68
1:A:640:TYR:CZ	1:A:644:LEU:HD11	2.28	0.68
1:A:446:LEU:O	1:A:450:VAL:HG12	1.93	0.68
1:A:31:TYR:HB3	1:A:35:ARG:NH2	2.09	0.68
1:A:1214:PHE:CE2	1:A:1222:LEU:HD21	2.30	0.67
1:A:1046:LYS:HG3	1:A:1048:ILE:HG22	1.76	0.67
1:A:609:THR:HG23	1:A:1327:ILE:HD12	1.77	0.67
1:A:575:ILE:HD11	1:A:603:ILE:HD13	1.76	0.67
1:A:381:LYS:HZ2	1:A:416:ILE:HG12	1.59	0.66
1:A:1289:LEU:HB2	1:A:1294:VAL:HB	1.76	0.66
1:A:1170:ILE:HG23	1:A:1176:ILE:HG21	1.77	0.66
1:A:310:PRO:HB2	1:A:313:LEU:HD13	1.78	0.66
1:A:1399:THR:HB	1:A:1402:GLU:HG3	1.78	0.66
1:A:1419:GLY:HA3	1:A:1452:ILE:HD11	1.77	0.65
1:A:668:THR:O	1:A:671:LEU:HG	1.95	0.65
1:A:122:VAL:HG22	1:A:445:LYS:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HB3	1:A:332:ILE:HG12	1.78	0.65
1:A:1135:VAL:HG12	1:A:1296:MET:HE2	1.80	0.64
1:A:42:CYS:O	1:A:45:ILE:HG12	1.98	0.64
1:A:109:GLU:O	1:A:112:LYS:HG2	1.98	0.64
1:A:486:VAL:O	1:A:489:ILE:HG12	1.99	0.63
1:A:725:GLU:HA	1:A:1396:MET:SD	2.38	0.63
1:A:304:TYR:HA	1:A:305:PRO:C	2.22	0.63
1:A:71:ASN:HD21	1:A:74:ALA:H	1.47	0.63
1:A:1056:ILE:HD12	1:A:1056:ILE:H	1.61	0.62
1:A:1369:ILE:H	1:A:1369:ILE:HD12	1.63	0.62
1:A:147:LEU:HD22	1:A:298:TYR:HB3	1.80	0.62
1:A:321:LEU:HD13	1:A:330:LEU:HD12	1.82	0.62
1:A:609:THR:HG21	1:A:1382:ILE:CG2	2.30	0.62
1:A:104:PRO:O	1:A:108:ARG:HG3	1.99	0.62
1:A:1272:ASP:HB3	1:A:1275:ILE:HG22	1.81	0.61
1:A:44:LEU:O	1:A:48:LEU:HD23	2.00	0.61
1:A:367:LEU:HA	1:A:370:GLU:HG2	1.82	0.61
1:A:1194:MET:HG3	1:A:1286:ILE:HG22	1.82	0.61
1:A:301:ASP:HB3	1:A:1254:LEU:HD21	1.83	0.60
1:A:107:LEU:HD23	1:A:376:ILE:HG23	1.83	0.60
1:A:1435:ASP:O	1:A:1438:VAL:HG12	2.02	0.60
1:A:8:HIS:CE1	1:A:11:LYS:HZ1	2.20	0.60
1:A:47:CYS:SG	1:A:537:LEU:HD12	2.41	0.60
1:A:357:TYR:CD2	1:A:395:LYS:HG2	2.36	0.60
1:A:1150:GLU:O	1:A:1151:LYS:C	2.43	0.60
1:A:517:THR:HG21	1:A:1054:GLY:O	2.01	0.60
1:A:1076:PHE:CE2	1:A:1080:ILE:HD11	2.37	0.59
1:A:375:TYR:HB2	1:A:378:TYR:CD2	2.37	0.59
1:A:1177:ASN:ND2	1:A:1295:GLN:H	1.95	0.59
1:A:1347:ILE:HG13	1:A:1459:LEU:HD13	1.84	0.59
1:A:31:TYR:HB3	1:A:35:ARG:HH22	1.66	0.59
1:A:1094:TYR:CE2	1:A:1098:LEU:HD11	2.38	0.59
1:A:643:VAL:HG13	1:A:647:LEU:HD23	1.85	0.59
1:A:324:VAL:HG21	1:A:438:TYR:CE1	2.37	0.59
1:A:1146:TYR:O	1:A:1149:LEU:HG	2.03	0.59
1:A:28:TYR:HA	1:A:31:TYR:HD2	1.67	0.59
1:A:1356:PHE:O	1:A:1359:MET:HG2	2.02	0.59
1:A:127:ILE:HD11	1:A:347:TYR:HE2	1.67	0.58
1:A:1064:VAL:HG12	1:A:1069:VAL:HG23	1.85	0.58
1:A:1339:TYR:O	1:A:1342:VAL:HG22	2.03	0.58
1:A:1060:PHE:HE2	1:A:1412:ILE:HG23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:O	1:A:146:GLU:HG3	2.02	0.58
1:A:1344:ILE:HG12	1:A:1389:VAL:HG21	1.85	0.58
1:A:407:VAL:HB	1:A:419:SER:HB3	1.86	0.58
1:A:166:GLY:HA2	1:A:169:PHE:CD2	2.39	0.57
1:A:488:ARG:O	1:A:491:LYS:HG2	2.04	0.57
1:A:1247:PHE:CZ	2:A:1501:CLR:H14	2.39	0.57
1:A:103:LYS:HD3	1:A:105:LYS:NZ	2.19	0.57
1:A:309:ILE:O	1:A:310:PRO:C	2.48	0.57
1:A:28:TYR:HA	1:A:31:TYR:CD2	2.39	0.57
1:A:301:ASP:HA	1:A:1255:ASN:HD21	1.69	0.57
1:A:84:PHE:HA	1:A:311:PRO:HD2	1.88	0.56
1:A:123:ASP:OD1	1:A:126:GLU:HG3	2.04	0.56
1:A:50:LEU:HD12	1:A:545:PHE:HB2	1.88	0.56
1:A:508:PHE:CZ	1:A:529:VAL:HG22	2.41	0.56
1:A:82:ASN:HD22	1:A:82:ASN:N	2.03	0.56
1:A:510:TYR:OH	1:A:1417:HIS:HA	2.05	0.56
1:A:366:PHE:HA	1:A:369:TYR:HD2	1.71	0.56
1:A:669:PHE:O	1:A:673:ARG:HG3	2.07	0.55
1:A:1207:VAL:HG12	1:A:1265:TYR:HB2	1.89	0.55
1:A:1336:LYS:HD2	1:A:1394:HIS:CE1	2.42	0.55
1:A:152:ILE:HA	1:A:309:ILE:HD11	1.89	0.55
1:A:32:VAL:HA	1:A:39:PHE:CE1	2.42	0.55
1:A:545:PHE:CE2	1:A:549:LEU:HD11	2.42	0.55
1:A:502:ILE:O	1:A:506:LEU:HG	2.07	0.54
1:A:1392:PHE:HZ	1:A:1400:ARG:HG3	1.73	0.54
1:A:1063:LEU:HD12	1:A:1067:TYR:CD1	2.43	0.54
1:A:1379:GLY:O	1:A:1382:ILE:HG22	2.07	0.54
1:A:14:LYS:HE3	1:A:1333:TYR:O	2.07	0.54
1:A:151:LEU:HD23	1:A:154:ARG:HH11	1.71	0.54
1:A:1226:ASN:HB3	1:A:1229:GLU:HB3	1.90	0.54
1:A:387:PHE:CD2	2:A:1501:CLR:H231	2.42	0.54
1:A:1218:ASN:O	1:A:1222:LEU:HD13	2.08	0.54
1:A:31:TYR:HB3	1:A:35:ARG:CZ	2.37	0.54
1:A:384:ASN:HD21	1:A:386:ASP:HB2	1.72	0.54
1:A:730:LEU:CD1	1:A:1049:TYR:HB3	2.38	0.54
1:A:1400:ARG:HD3	1:A:1467:GLY:N	2.13	0.54
1:A:129:GLU:HG3	1:A:437:PRO:HB3	1.89	0.54
1:A:1312:ILE:HG23	1:A:1366:MET:HE2	1.89	0.54
1:A:123:ASP:CG	1:A:126:GLU:HG3	2.33	0.53
1:A:1141:HIS:NE2	1:A:1178:LYS:HG3	2.23	0.53
1:A:1214:PHE:CE1	1:A:1234:PHE:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:SER:O	1:A:1460:PRO:HG2	2.07	0.53
1:A:459:ILE:HD13	1:A:472:ILE:HG22	1.90	0.53
1:A:1149:LEU:CD1	1:A:1150:GLU:HG2	2.38	0.53
1:A:13:LEU:HA	1:A:16:LYS:HE2	1.90	0.53
1:A:731:TYR:CE1	1:A:1405:LYS:HE2	2.44	0.53
1:A:455:LEU:O	1:A:458:ILE:HG22	2.09	0.52
1:A:447:ILE:O	1:A:451:ARG:HG3	2.10	0.52
1:A:365:LEU:HD13	1:A:403:LEU:HD11	1.91	0.52
1:A:1423:TRP:HA	1:A:1426:ILE:HG12	1.90	0.52
1:A:3:VAL:O	1:A:7:ILE:HG13	2.10	0.52
1:A:306:TYR:C	1:A:308:TYR:H	2.17	0.52
1:A:485:GLU:O	1:A:489:ILE:HG23	2.08	0.52
1:A:1390:GLN:HG3	1:A:1394:HIS:HD2	1.75	0.52
1:A:390:ASN:HB3	1:A:393:THR:HG1	1.75	0.52
1:A:545:PHE:O	1:A:549:LEU:HG	2.10	0.52
1:A:140:GLN:HB3	1:A:145:LYS:CD	2.39	0.51
1:A:371:LYS:CB	1:A:392:ARG:HB2	2.40	0.51
1:A:1331:THR:O	1:A:1334:ILE:HG13	2.10	0.51
1:A:1052:PRO:HD2	1:A:1055:ASN:ND2	2.25	0.51
1:A:94:LEU:HD13	1:A:424:MET:HB2	1.92	0.51
1:A:123:ASP:HA	1:A:346:THR:HG22	1.92	0.51
1:A:1184:ASN:HB3	1:A:1186:ASN:OD1	2.11	0.51
1:A:31:TYR:HB3	1:A:35:ARG:NH1	2.25	0.51
1:A:516:VAL:HA	1:A:523:SER:HB2	1.92	0.51
1:A:390:ASN:HB3	1:A:393:THR:OG1	2.11	0.51
1:A:357:TYR:HD2	1:A:395:LYS:HG2	1.72	0.51
1:A:1289:LEU:H	1:A:1289:LEU:HD22	1.76	0.51
1:A:147:LEU:HD23	1:A:313:LEU:HD21	1.91	0.51
1:A:373:ASN:HA	1:A:392:ARG:CZ	2.41	0.51
1:A:103:LYS:HD3	1:A:105:LYS:HZ3	1.74	0.50
1:A:606:THR:HG23	1:A:1383:ASP:CG	2.36	0.50
1:A:384:ASN:HA	1:A:415:TYR:HE2	1.75	0.50
1:A:140:GLN:HG2	1:A:144:ALA:HB3	1.93	0.50
1:A:1076:PHE:O	1:A:1080:ILE:HG13	2.11	0.50
1:A:71:ASN:ND2	1:A:74:ALA:H	2.10	0.50
1:A:80:THR:CA	1:A:1147:ARG:HH21	2.16	0.50
1:A:583:PHE:CE2	1:A:1051:GLU:HG2	2.47	0.50
1:A:385:LEU:HG	1:A:415:TYR:CD2	2.47	0.50
1:A:1390:GLN:HG3	1:A:1394:HIS:CD2	2.46	0.50
1:A:1457:MET:C	1:A:1460:PRO:HD2	2.37	0.50
1:A:325:PHE:CE1	1:A:352:ILE:HG23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:CD1	1:A:631:PHE:HA	2.42	0.49
1:A:588:ASN:OD1	1:A:659:LYS:HB2	2.12	0.49
1:A:4:LYS:HD3	1:A:4:LYS:C	2.37	0.49
1:A:1277:SER:O	1:A:1281:LYS:HG3	2.12	0.49
1:A:1339:TYR:CE2	1:A:1343:ILE:HD11	2.47	0.49
1:A:1084:MET:O	1:A:1087:ILE:HG22	2.12	0.49
1:A:1132:PHE:CZ	2:A:1501:CLR:H21	2.47	0.49
1:A:1267:GLN:NE2	1:A:1279:TRP:HE3	2.09	0.49
1:A:1366:MET:HB2	1:A:1371:MET:SD	2.52	0.49
1:A:305:PRO:HB2	1:A:307:GLN:CD	2.37	0.49
1:A:1104:LYS:HB2	1:A:1107:LYS:HZ3	1.76	0.49
1:A:1339:TYR:O	1:A:1343:ILE:HG13	2.13	0.49
1:A:373:ASN:OD1	1:A:390:ASN:HA	2.13	0.49
1:A:527:CYS:SG	1:A:651:LEU:HA	2.53	0.49
1:A:622:PHE:HZ	1:A:1308:THR:HB	1.76	0.49
1:A:1084:MET:O	1:A:1088:ILE:HG13	2.13	0.49
1:A:50:LEU:O	1:A:544:GLY:HA3	2.12	0.49
1:A:124:LEU:HA	1:A:127:ILE:HD13	1.94	0.49
1:A:35:ARG:HG3	1:A:39:PHE:CE1	2.48	0.49
1:A:41:ILE:HG13	1:A:42:CYS:N	2.27	0.49
1:A:1189:GLU:O	1:A:1192:ILE:HG22	2.12	0.49
1:A:1242:PHE:O	1:A:1246:LEU:HG	2.12	0.49
1:A:106:ILE:HG22	1:A:110:LEU:HD23	1.95	0.48
1:A:1126:PHE:HB3	1:A:1129:PHE:HD2	1.78	0.48
1:A:1339:TYR:CD2	1:A:1468:PRO:HG3	2.48	0.48
1:A:1459:LEU:HB3	1:A:1460:PRO:HD3	1.94	0.48
1:A:1085:PHE:CZ	1:A:1453:THR:HG22	2.47	0.48
1:A:131:LYS:O	1:A:335:ARG:HA	2.13	0.48
1:A:1270:VAL:HG21	1:A:1275:ILE:HG21	1.95	0.48
1:A:1399:THR:H	1:A:1402:GLU:CD	2.20	0.48
1:A:339:ASP:HB3	1:A:343:LYS:NZ	2.29	0.48
1:A:390:ASN:O	1:A:394:TYR:N	2.45	0.48
1:A:1057:GLY:O	1:A:1061:ARG:HG3	2.13	0.48
1:A:41:ILE:O	1:A:45:ILE:HG23	2.13	0.48
1:A:572:VAL:HG22	1:A:647:LEU:HD22	1.95	0.48
1:A:1229:GLU:O	1:A:1233:ILE:HG12	2.13	0.48
1:A:1385:THR:HG23	1:A:1459:LEU:HD22	1.96	0.48
1:A:1142:PHE:CD1	1:A:1254:LEU:HD12	2.48	0.48
1:A:1352:ASP:HA	1:A:1355:ILE:HG12	1.95	0.48
1:A:58:GLU:OE1	1:A:552:LYS:HE2	2.14	0.48
1:A:105:LYS:HE2	1:A:458:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:ASP:O	1:A:1113:SER:C	2.56	0.48
1:A:98:ASN:HD21	1:A:470:PRO:HA	1.77	0.48
1:A:1078:LYS:O	1:A:1079:THR:C	2.57	0.48
1:A:612:ILE:O	1:A:616:ILE:HG12	2.14	0.47
1:A:1356:PHE:HA	1:A:1359:MET:HE3	1.95	0.47
1:A:441:ALA:O	1:A:445:LYS:HG2	2.14	0.47
1:A:1318:ILE:O	1:A:1322:ILE:HG13	2.13	0.47
1:A:62:ASP:CG	1:A:65:LYS:HB3	2.40	0.47
1:A:1132:PHE:HZ	2:A:1501:CLR:H21	1.80	0.47
1:A:1323:THR:O	1:A:1324:ILE:C	2.57	0.47
1:A:71:ASN:ND2	1:A:73:TYR:HB3	2.29	0.47
1:A:508:PHE:CZ	1:A:529:VAL:HG13	2.49	0.47
1:A:727:ILE:HD12	1:A:730:LEU:HD23	1.97	0.47
1:A:97:SER:OG	1:A:99:VAL:HG22	2.14	0.47
1:A:302:VAL:H	1:A:1255:ASN:ND2	2.12	0.47
1:A:508:PHE:HZ	1:A:529:VAL:HG13	1.80	0.47
1:A:174:LEU:HB3	1:A:178:GLY:HA2	1.95	0.47
1:A:1176:ILE:HG23	1:A:1295:GLN:HB3	1.97	0.47
1:A:141:SER:O	1:A:144:ALA:HB3	2.15	0.47
1:A:328:LYS:C	1:A:330:LEU:N	2.72	0.47
1:A:575:ILE:HD11	1:A:603:ILE:HG21	1.97	0.47
1:A:1174:PRO:O	1:A:1178:LYS:HD3	2.15	0.47
1:A:9:LYS:O	1:A:12:GLU:HB3	2.15	0.46
1:A:45:ILE:HG13	1:A:46:CYS:N	2.30	0.46
1:A:110:LEU:O	1:A:113:PHE:HB3	2.16	0.46
1:A:156:GLU:O	1:A:160:LYS:HG3	2.15	0.46
1:A:546:LEU:HD12	1:A:631:PHE:HA	1.96	0.46
1:A:1076:PHE:CZ	1:A:1080:ILE:HD11	2.50	0.46
1:A:1149:LEU:C	1:A:1149:LEU:HD12	2.40	0.46
1:A:8:HIS:HA	1:A:11:LYS:HD3	1.97	0.46
1:A:444:LYS:O	1:A:447:ILE:HG12	2.16	0.46
1:A:143:VAL:HA	1:A:146:GLU:CD	2.41	0.46
1:A:402:ILE:HB	1:A:403:LEU:HD12	1.97	0.46
1:A:539:PHE:HD2	1:A:540:LEU:HD23	1.81	0.46
1:A:578:SER:O	1:A:582:LEU:HD23	2.14	0.46
1:A:456:ASP:O	1:A:459:ILE:HG12	2.15	0.46
1:A:1313:ILE:O	1:A:1317:LEU:HG	2.15	0.46
1:A:319:CYS:SG	1:A:335:ARG:HD3	2.56	0.46
1:A:130:CYS:SG	1:A:319:CYS:HA	2.56	0.46
1:A:359:ASP:O	1:A:360:CYS:C	2.58	0.46
1:A:530:MET:HG3	1:A:650:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:PHE:CE1	1:A:641:LEU:HD21	2.50	0.46
1:A:1059:TYR:O	1:A:1060:PHE:C	2.59	0.46
1:A:457:ASP:HA	1:A:460:GLN:NE2	2.31	0.46
1:A:517:THR:OG1	1:A:1054:GLY:HA2	2.16	0.46
1:A:1139:ASP:O	1:A:1143:ILE:HG12	2.16	0.46
1:A:1200:SER:O	1:A:1201:GLN:C	2.59	0.46
1:A:65:LYS:HE2	1:A:623:TYR:CG	2.51	0.46
1:A:122:VAL:HG13	1:A:126:GLU:OE1	2.15	0.46
1:A:339:ASP:O	1:A:343:LYS:HG3	2.15	0.46
1:A:546:LEU:HD12	1:A:631:PHE:CD1	2.50	0.46
1:A:57:LYS:HE2	1:A:59:HIS:CE1	2.51	0.46
1:A:20:LYS:O	1:A:24:LEU:HG	2.15	0.46
1:A:371:LYS:CG	1:A:393:THR:HG22	2.46	0.46
1:A:1398:ARG:HG3	1:A:1402:GLU:OE1	2.16	0.45
1:A:40:ILE:HD13	1:A:650:PHE:CE1	2.50	0.45
1:A:121:GLU:HG2	1:A:346:THR:HB	1.98	0.45
1:A:440:LEU:HB3	1:A:480:ARG:NH1	2.32	0.45
1:A:1068:TYR:OH	1:A:1457:MET:HG2	2.16	0.45
1:A:140:GLN:O	1:A:141:SER:C	2.58	0.45
1:A:408:TYR:HE2	1:A:410:LYS:HZ3	1.63	0.45
1:A:646:PHE:CZ	1:A:650:PHE:CE1	3.04	0.45
1:A:1201:GLN:HB3	1:A:1203:PHE:CE1	2.51	0.45
1:A:13:LEU:O	1:A:14:LYS:C	2.58	0.45
1:A:378:TYR:HB3	1:A:379:PRO:HD2	1.99	0.45
1:A:554:VAL:HB	1:A:556:PRO:HD2	1.99	0.45
1:A:1138:PHE:HB3	1:A:1143:ILE:HG13	1.99	0.45
1:A:632:THR:O	1:A:636:LEU:HG	2.17	0.45
1:A:1116:ARG:O	1:A:1120:THR:HG23	2.16	0.45
1:A:60:GLU:HG3	1:A:62:ASP:OD1	2.16	0.45
1:A:60:GLU:HB3	1:A:66:LEU:HD21	1.98	0.45
1:A:385:LEU:HD21	1:A:415:TYR:HB2	1.98	0.45
1:A:349:LEU:HD13	1:A:442:TYR:CE2	2.52	0.45
1:A:1367:ASN:O	1:A:1371:MET:HG2	2.16	0.45
1:A:1309:ASP:O	1:A:1312:ILE:HG22	2.17	0.44
1:A:321:LEU:CD2	1:A:328:LYS:HG3	2.47	0.44
1:A:365:LEU:HD11	1:A:380:ILE:HD13	1.99	0.44
1:A:1231:TYR:CD1	1:A:1256:GLY:HA2	2.53	0.44
1:A:501:LEU:O	1:A:505:LEU:HD13	2.18	0.44
1:A:1089:ILE:HD11	1:A:1350:LEU:HD21	2.00	0.44
1:A:1149:LEU:HD11	1:A:1150:GLU:HG2	1.99	0.44
1:A:1312:ILE:HD13	1:A:1366:MET:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ARG:HD2	1:A:1054:GLY:C	2.42	0.44
1:A:539:PHE:CD2	1:A:540:LEU:HD23	2.52	0.44
1:A:1055:ASN:O	1:A:1056:ILE:C	2.60	0.44
1:A:100:ASN:C	1:A:102:LEU:N	2.71	0.44
1:A:340:GLY:O	1:A:344:GLN:HG2	2.18	0.44
1:A:368:TYR:O	1:A:373:ASN:HB3	2.18	0.44
1:A:409:GLU:O	1:A:415:TYR:HA	2.18	0.44
1:A:492:ILE:N	1:A:492:ILE:HD12	2.31	0.44
1:A:533:PHE:O	1:A:534:CYS:C	2.61	0.44
1:A:312:MET:HE1	1:A:1147:ARG:HA	1.98	0.44
1:A:671:LEU:HD12	1:A:672:PHE:N	2.32	0.44
1:A:1140:LYS:NZ	1:A:1176:ILE:HB	2.32	0.44
1:A:1438:VAL:O	1:A:1442:GLN:HG3	2.18	0.44
1:A:1068:TYR:CZ	1:A:1072:LEU:HD11	2.53	0.44
1:A:1369:ILE:O	1:A:1373:ILE:HG12	2.18	0.44
1:A:321:LEU:HD22	1:A:328:LYS:HG3	2.00	0.43
1:A:1054:GLY:O	1:A:1055:ASN:C	2.59	0.43
1:A:325:PHE:HE1	1:A:352:ILE:HG23	1.83	0.43
1:A:1411:MET:C	1:A:1414:PRO:HD2	2.43	0.43
1:A:370:GLU:HB2	1:A:393:THR:HG21	1.99	0.43
1:A:371:LYS:HB3	1:A:392:ARG:HB2	2.00	0.43
1:A:456:ASP:O	1:A:460:GLN:HG3	2.18	0.43
1:A:607:THR:O	1:A:608:LEU:C	2.61	0.43
1:A:572:VAL:O	1:A:576:LEU:HG	2.18	0.43
1:A:1083:ILE:O	1:A:1086:THR:HB	2.18	0.43
1:A:1242:PHE:CE2	1:A:1246:LEU:HD11	2.54	0.43
1:A:1369:ILE:HD12	1:A:1369:ILE:N	2.32	0.43
1:A:45:ILE:O	1:A:49:LEU:HG	2.17	0.43
1:A:68:SER:HB2	1:A:1304:ILE:HG13	2.00	0.43
1:A:135:GLU:CD	1:A:135:GLU:H	2.27	0.43
1:A:1389:VAL:HG23	1:A:1459:LEU:HD21	2.00	0.43
1:A:664:ILE:HG23	1:A:665:PHE:N	2.33	0.43
1:A:1069:VAL:O	1:A:1070:PRO:C	2.59	0.43
1:A:1314:GLU:O	1:A:1315:VAL:C	2.61	0.43
1:A:387:PHE:CG	2:A:1501:CLR:H231	2.54	0.43
1:A:730:LEU:O	1:A:734:GLU:HG3	2.19	0.43
1:A:1430:PHE:HB2	1:A:1441:PHE:CE2	2.53	0.43
1:A:85:PHE:HZ	1:A:1261:TRP:HA	1.83	0.43
1:A:352:ILE:HG22	1:A:435:TYR:HD1	1.84	0.43
1:A:555:PRO:HB2	1:A:556:PRO:HD3	2.00	0.43
1:A:1340:SER:O	1:A:1344:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:HZ	1:A:1147:ARG:HG2	1.84	0.43
1:A:86:TYR:OH	1:A:314:ILE:HG13	2.18	0.43
1:A:341:LEU:HA	1:A:344:GLN:HG2	2.01	0.43
1:A:1210:GLY:O	1:A:1211:PHE:C	2.61	0.43
1:A:1351:ILE:HD13	1:A:1451:SER:HA	2.01	0.43
1:A:80:THR:HA	1:A:1147:ARG:NH2	2.17	0.42
1:A:563:LEU:O	1:A:564:VAL:C	2.62	0.42
1:A:1069:VAL:HB	1:A:1070:PRO:HD3	1.99	0.42
1:A:35:ARG:HG3	1:A:39:PHE:HE1	1.85	0.42
1:A:328:LYS:C	1:A:330:LEU:H	2.27	0.42
1:A:368:TYR:HB2	1:A:399:PHE:HZ	1.84	0.42
1:A:645:THR:O	1:A:646:PHE:C	2.60	0.42
1:A:727:ILE:O	1:A:730:LEU:HB3	2.19	0.42
1:A:1046:LYS:CG	1:A:1048:ILE:HG22	2.46	0.42
1:A:1278:LYS:HZ2	1:A:1279:TRP:CD1	2.36	0.42
1:A:1369:ILE:O	1:A:1372:VAL:HG12	2.18	0.42
1:A:1284:LYS:HB2	1:A:1284:LYS:HE3	1.80	0.42
1:A:493:ASP:O	1:A:497:ARG:HG3	2.19	0.42
1:A:1212:THR:O	1:A:1213:PHE:C	2.60	0.42
1:A:1289:LEU:N	1:A:1294:VAL:O	2.53	0.42
1:A:102:LEU:HG	1:A:420:ALA:HB3	2.01	0.42
1:A:317:ASP:OD1	1:A:323:ASN:ND2	2.53	0.42
1:A:565:ILE:O	1:A:569:VAL:HG23	2.19	0.42
1:A:99:VAL:HG12	1:A:463:GLU:O	2.20	0.42
1:A:1403:LYS:HE2	1:A:1469:LEU:HD12	2.00	0.42
1:A:146:GLU:HA	1:A:149:LYS:HE3	2.00	0.42
1:A:175:ASP:CG	1:A:176:GLU:N	2.77	0.42
1:A:1170:ILE:O	1:A:1176:ILE:HG13	2.20	0.42
1:A:1331:THR:HG21	1:A:1382:ILE:HG12	2.02	0.42
1:A:57:LYS:HE2	1:A:59:HIS:NE2	2.34	0.42
1:A:57:LYS:HG3	1:A:547:TYR:CE1	2.55	0.42
1:A:388:TYR:HB3	1:A:399:PHE:CE1	2.54	0.42
1:A:400:LYS:HE3	1:A:400:LYS:HB2	1.79	0.42
1:A:450:VAL:HG11	1:A:476:VAL:HB	2.02	0.42
1:A:130:CYS:HB3	1:A:334:LEU:HB2	2.02	0.42
1:A:367:LEU:HA	1:A:370:GLU:CG	2.50	0.42
1:A:560:VAL:HB	1:A:561:PRO:HD3	2.02	0.42
1:A:1248:LYS:HG3	1:A:1249:ASN:OD1	2.20	0.42
1:A:11:LYS:HG2	1:A:12:GLU:N	2.34	0.41
1:A:610:ASN:O	1:A:614:PHE:HD2	2.03	0.41
1:A:614:PHE:CE1	1:A:1376:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HA	1:A:154:ARG:HG2	2.02	0.41
1:A:295:PHE:O	1:A:296:THR:C	2.63	0.41
1:A:318:ARG:HD2	1:A:437:PRO:HG2	2.01	0.41
1:A:128:ASN:O	1:A:129:GLU:C	2.64	0.41
1:A:128:ASN:OD1	1:A:131:LYS:HD3	2.20	0.41
1:A:349:LEU:HD22	1:A:442:TYR:OH	2.20	0.41
1:A:371:LYS:HB2	1:A:392:ARG:HB2	2.01	0.41
1:A:349:LEU:HD21	1:A:427:ILE:HG21	2.03	0.41
1:A:387:PHE:CE2	2:A:1501:CLR:H272	2.55	0.41
1:A:539:PHE:CZ	1:A:561:PRO:HG3	2.55	0.41
1:A:1226:ASN:HB3	1:A:1229:GLU:CB	2.50	0.41
1:A:339:ASP:HA	1:A:342:LYS:HE2	2.01	0.41
1:A:1149:LEU:HD12	1:A:1150:GLU:N	2.35	0.41
1:A:1171:MET:O	1:A:1172:ASN:C	2.63	0.41
1:A:299:LYS:HG2	1:A:300:ASP:OD1	2.20	0.41
1:A:14:LYS:O	1:A:18:LEU:HG	2.21	0.41
1:A:356:LYS:HG2	1:A:357:TYR:CD2	2.55	0.41
1:A:526:LEU:HB3	1:A:654:GLU:OE1	2.20	0.41
1:A:534:CYS:SG	1:A:642:MET:CB	3.09	0.41
1:A:1176:ILE:HD13	1:A:1176:ILE:HA	1.93	0.41
1:A:1240:LYS:O	1:A:1241:ASP:C	2.60	0.41
1:A:124:LEU:HB2	1:A:342:LYS:O	2.20	0.41
1:A:164:ILE:N	1:A:164:ILE:HD12	2.36	0.41
1:A:171:TYR:CE2	1:A:1228:GLN:HB2	2.56	0.41
1:A:328:LYS:HB3	1:A:330:LEU:CG	2.48	0.41
1:A:664:ILE:HG23	1:A:665:PHE:H	1.85	0.41
1:A:1316:THR:HG21	1:A:1371:MET:HE3	2.02	0.41
1:A:1339:TYR:HD2	1:A:1468:PRO:HG3	1.86	0.41
1:A:154:ARG:NH2	1:A:300:ASP:HA	2.36	0.41
1:A:347:TYR:OH	1:A:441:ALA:HB3	2.21	0.41
1:A:482:LEU:O	1:A:486:VAL:HG23	2.20	0.41
1:A:512:LEU:O	1:A:516:VAL:HG22	2.21	0.41
1:A:526:LEU:HB3	1:A:654:GLU:CD	2.45	0.41
1:A:670:HIS:HA	1:A:673:ARG:HH11	1.85	0.41
1:A:1187:LEU:HB2	1:A:1292:HIS:CD2	2.56	0.41
1:A:1301:LEU:C	1:A:1301:LEU:HD23	2.46	0.41
1:A:1173:SER:HB3	1:A:1176:ILE:CG1	2.47	0.41
1:A:1195:HIS:CD2	1:A:1212:THR:HG21	2.55	0.41
1:A:74:ALA:O	1:A:77:THR:HB	2.21	0.40
1:A:1061:ARG:O	1:A:1062:SER:C	2.63	0.40
1:A:1304:ILE:HG23	1:A:1305:PHE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HB2	1:A:442:TYR:CZ	2.56	0.40
1:A:388:TYR:HB3	1:A:399:PHE:HE1	1.86	0.40
1:A:494:ASN:HA	1:A:497:ARG:HD2	2.04	0.40
1:A:1427:SER:HA	1:A:1441:PHE:CE1	2.55	0.40
1:A:36:PRO:HG3	1:A:656:LYS:NZ	2.36	0.40
1:A:84:PHE:CE2	1:A:1143:ILE:HG23	2.56	0.40
2:A:1501:CLR:H162	2:A:1501:CLR:H222	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	975/1470 (66%)	931 (96%)	43 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	905/1371 (66%)	897 (99%)	8 (1%)	70 78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	177	ASN
1	A	352	ILE
1	A	450	VAL
1	A	733	PHE
1	A	1254	LEU
1	A	1342	VAL
1	A	1466	PHE

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	8	HIS
1	A	15	GLN
1	A	23	ASN
1	A	78	ASN
1	A	82	ASN
1	A	140	GLN
1	A	431	ASN
1	A	433	HIS
1	A	514	ASN
1	A	588	ASN
1	A	1177	ASN
1	A	1201	GLN
1	A	1255	ASN
1	A	1267	GLN
1	A	1269	ASN
1	A	1291	ASN
1	A	1293	ASN
1	A	1442	GLN

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1502	1	14,14,15	0.30	0	17,19,21	0.63	0
2	CLR	A	1501	-	31,31,31	0.88	2 (6%)	48,48,48	1.36	8 (16%)
3	NAG	A	1503	1	14,14,15	0.33	0	17,19,21	1.47	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1502	1	-	2/6/23/26	0/1/1/1
2	CLR	A	1501	-	-	0/10/68/68	0/4/4/4
3	NAG	A	1503	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	CLR	C13-C14	-2.17	1.51	1.55
2	A	1501	CLR	C10-C9	-2.14	1.52	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	NAG	C1-O5-C5	4.95	118.82	112.19
2	A	1501	CLR	C13-C14-C8	-3.16	109.92	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	CLR	C11-C12-C13	-2.89	107.87	112.74
2	A	1501	CLR	C8-C7-C6	-2.86	108.79	112.76
2	A	1501	CLR	C17-C13-C14	2.85	103.37	100.10
2	A	1501	CLR	C13-C17-C20	-2.76	115.23	119.50
2	A	1501	CLR	C11-C9-C10	-2.47	110.04	113.08
2	A	1501	CLR	C3-C4-C5	-2.15	108.62	112.05
2	A	1501	CLR	C19-C10-C9	-2.15	109.25	111.66
3	A	1503	NAG	C4-C3-C2	-2.01	108.07	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

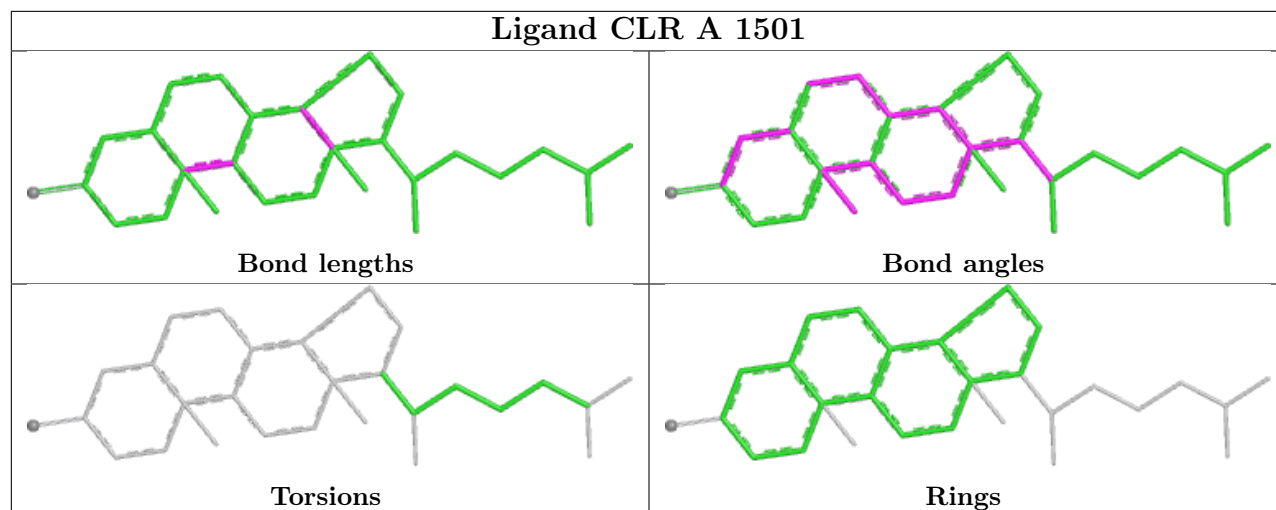
Mol	Chain	Res	Type	Atoms
3	A	1502	NAG	C8-C7-N2-C2
3	A	1502	NAG	O7-C7-N2-C2
3	A	1503	NAG	C8-C7-N2-C2
3	A	1503	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	NAG	1	0
2	A	1501	CLR	7	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

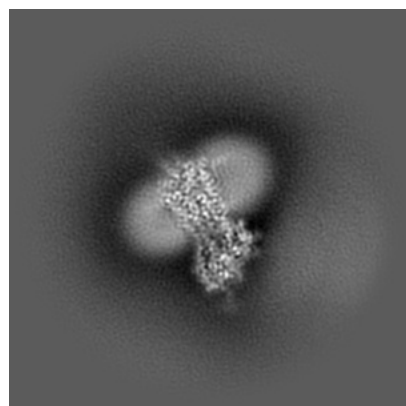
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42854. These allow visual inspection of the internal detail of the map and identification of artifacts.

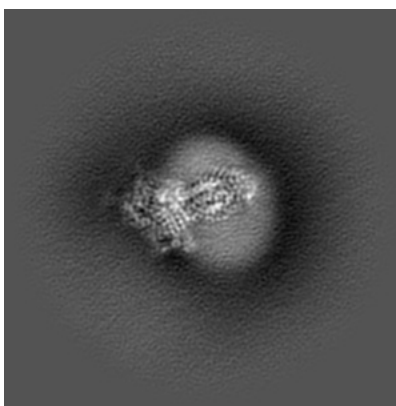
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

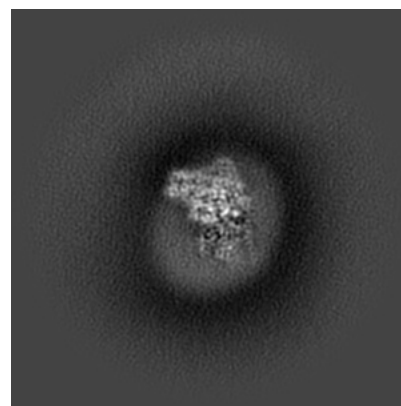
6.1.1 Primary map



X

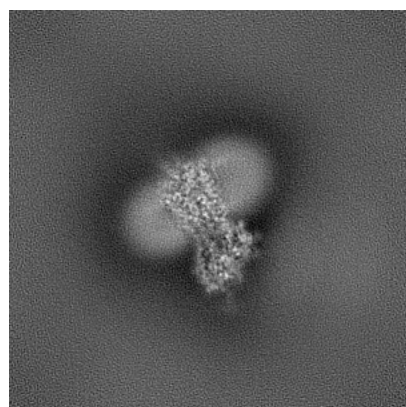


Y

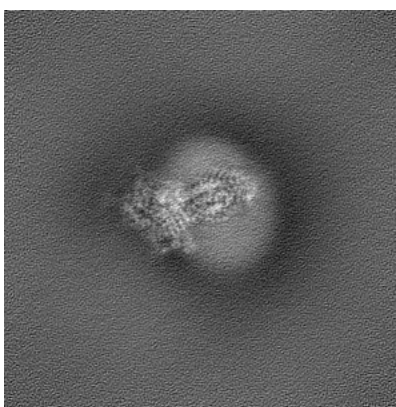


Z

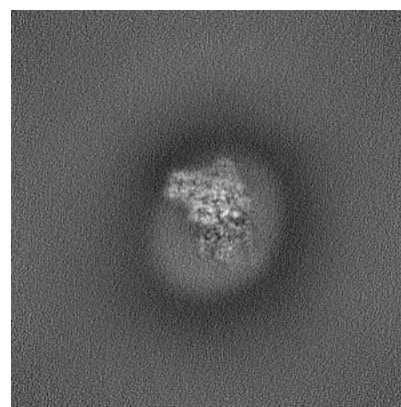
6.1.2 Raw map



X



Y

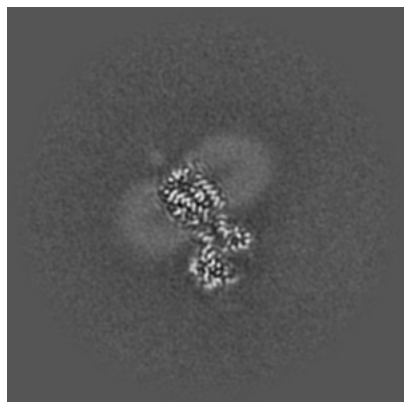


Z

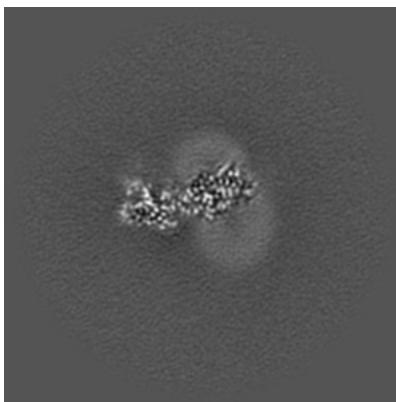
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

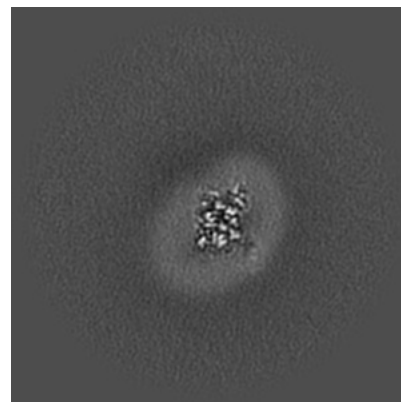
6.2.1 Primary map



X Index: 150

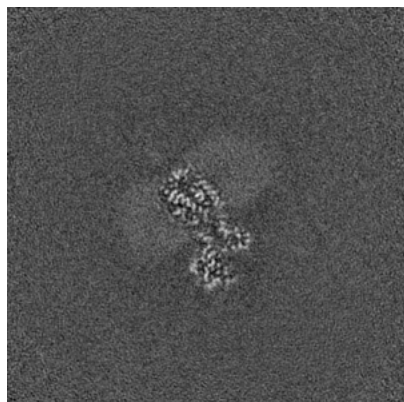


Y Index: 150

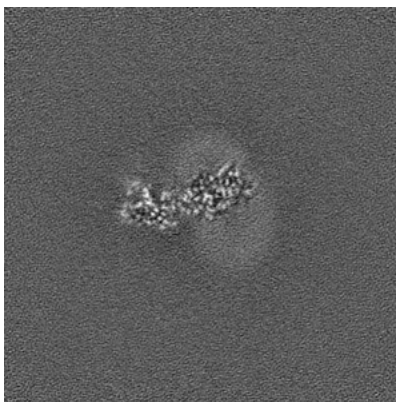


Z Index: 150

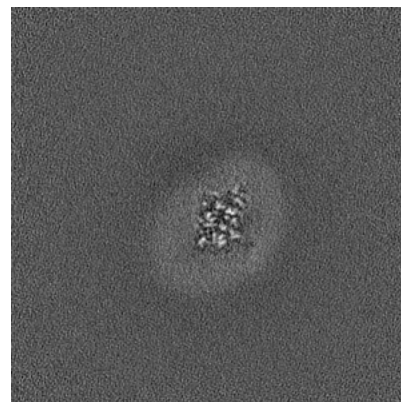
6.2.2 Raw map



X Index: 150



Y Index: 150

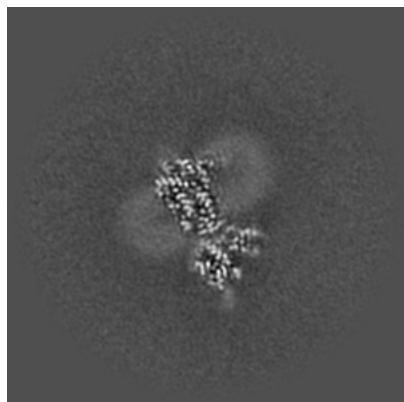


Z Index: 150

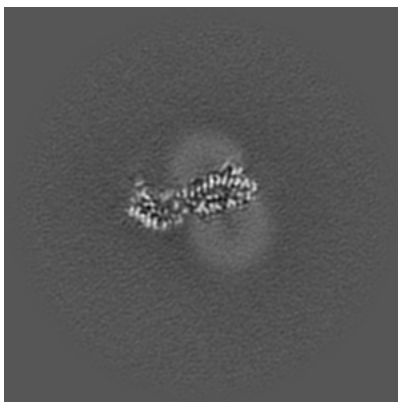
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

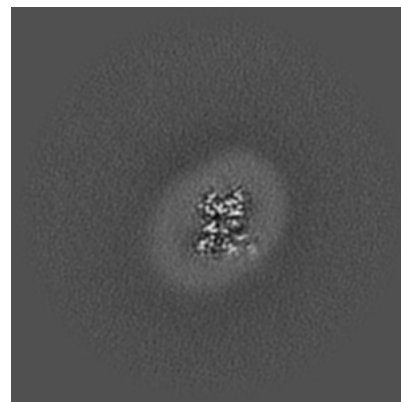
6.3.1 Primary map



X Index: 158

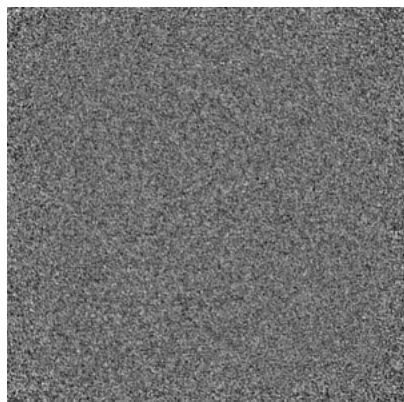


Y Index: 145

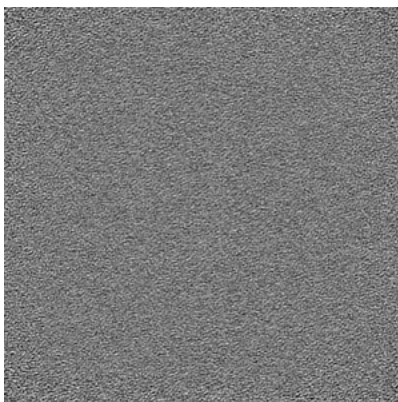


Z Index: 155

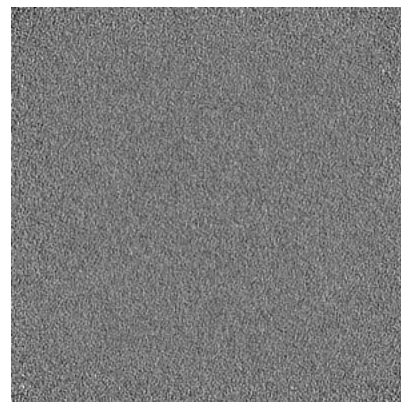
6.3.2 Raw map



X Index: 0



Y Index: 0

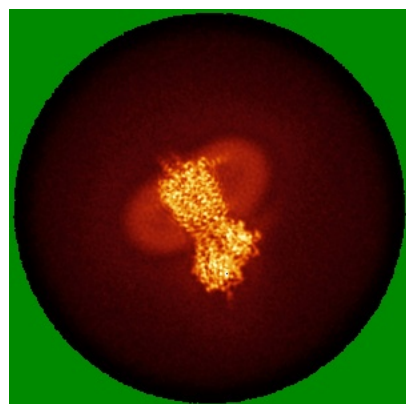


Z Index: 0

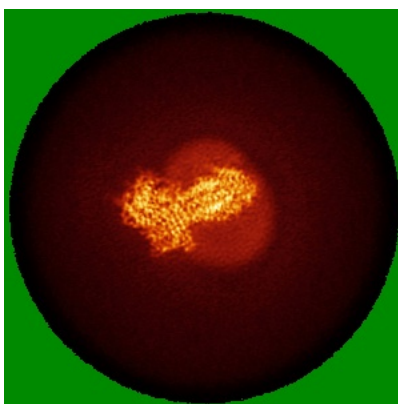
The images above show the largest variance slices of the map in three orthogonal directions.

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

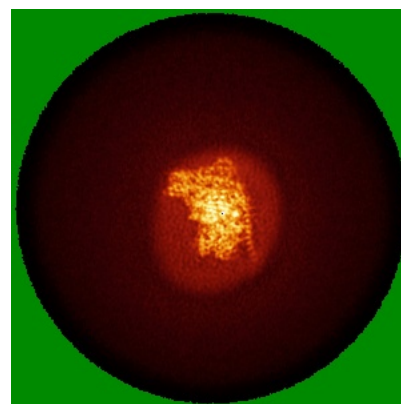
6.4.1 Primary map



X

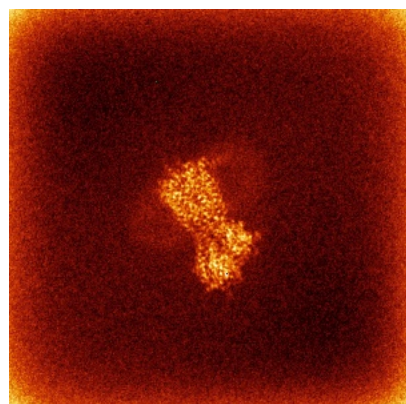


Y

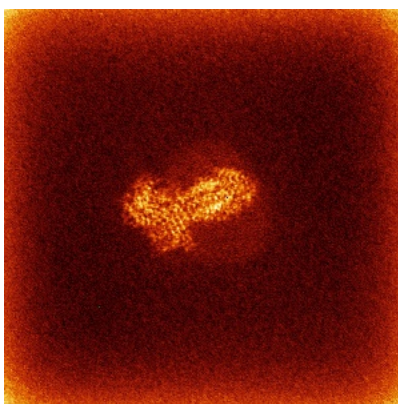


Z

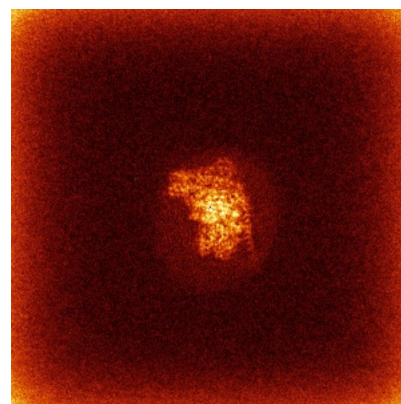
6.4.2 Raw map



X



Y

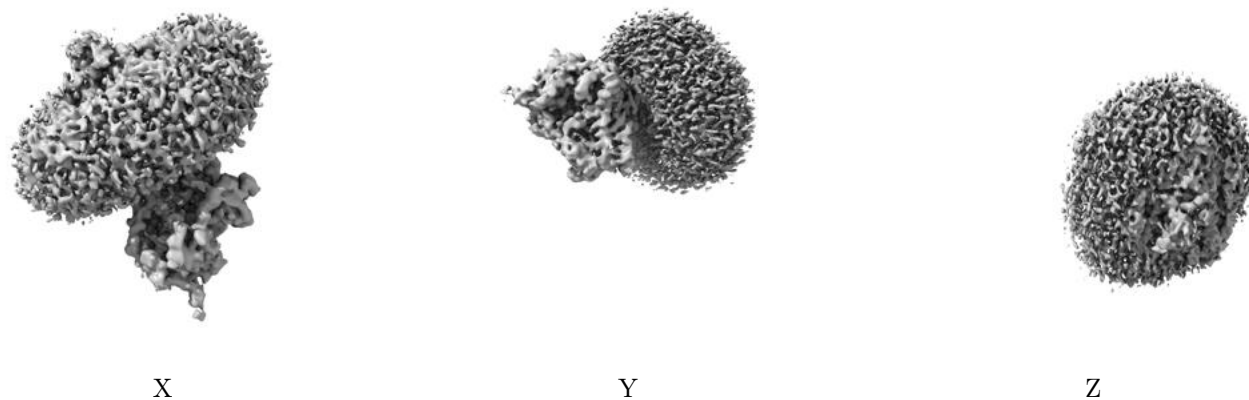


Z

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

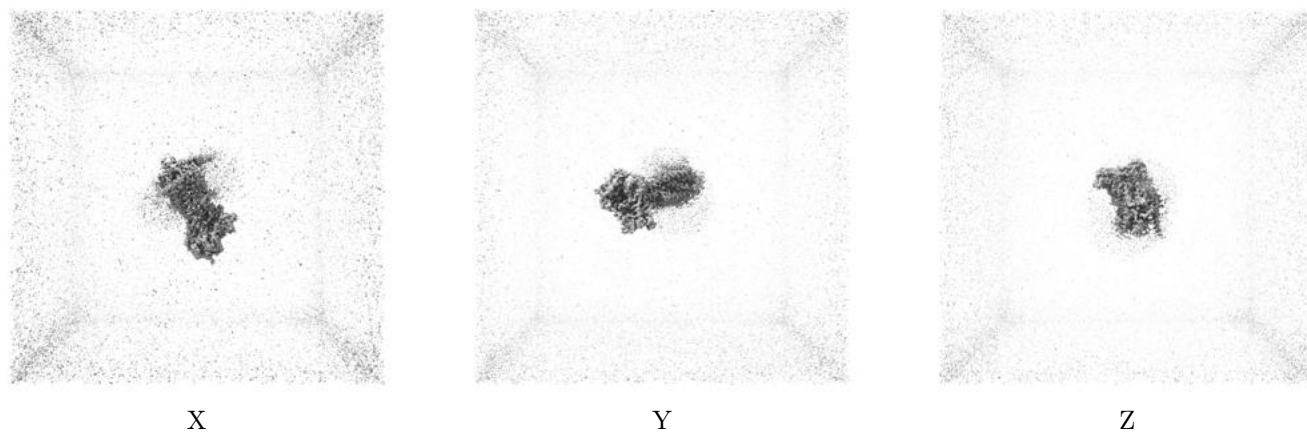
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

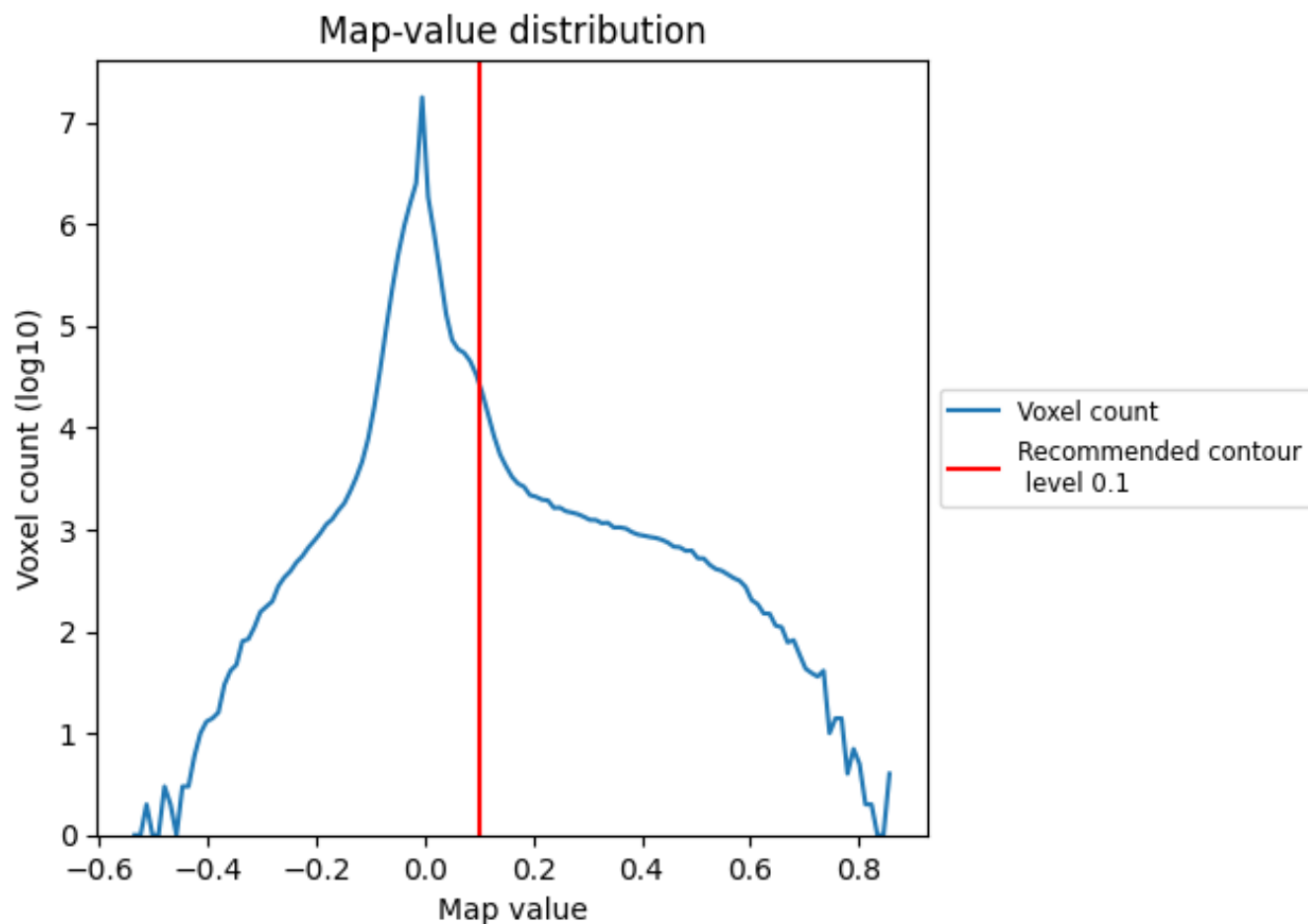
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

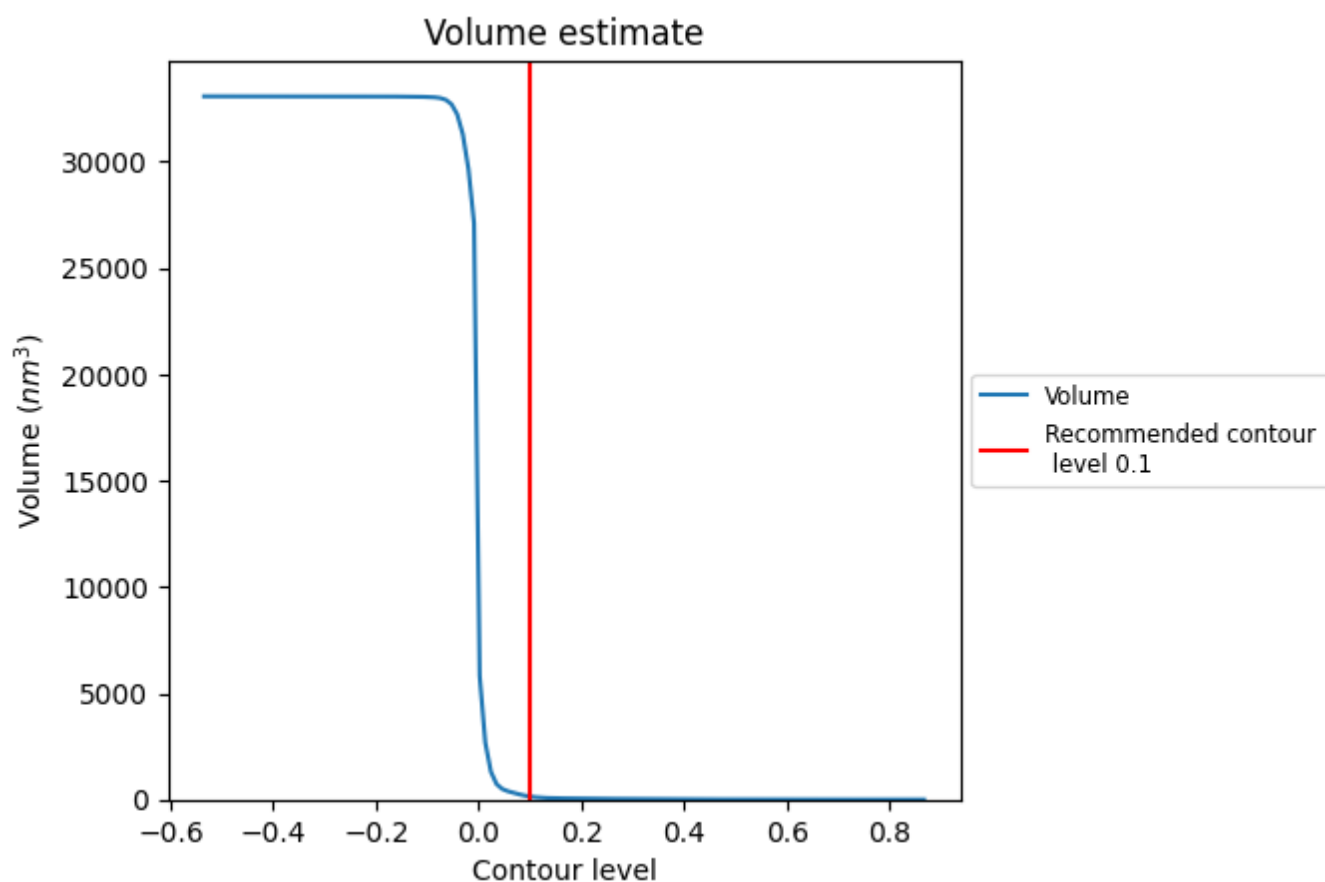
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

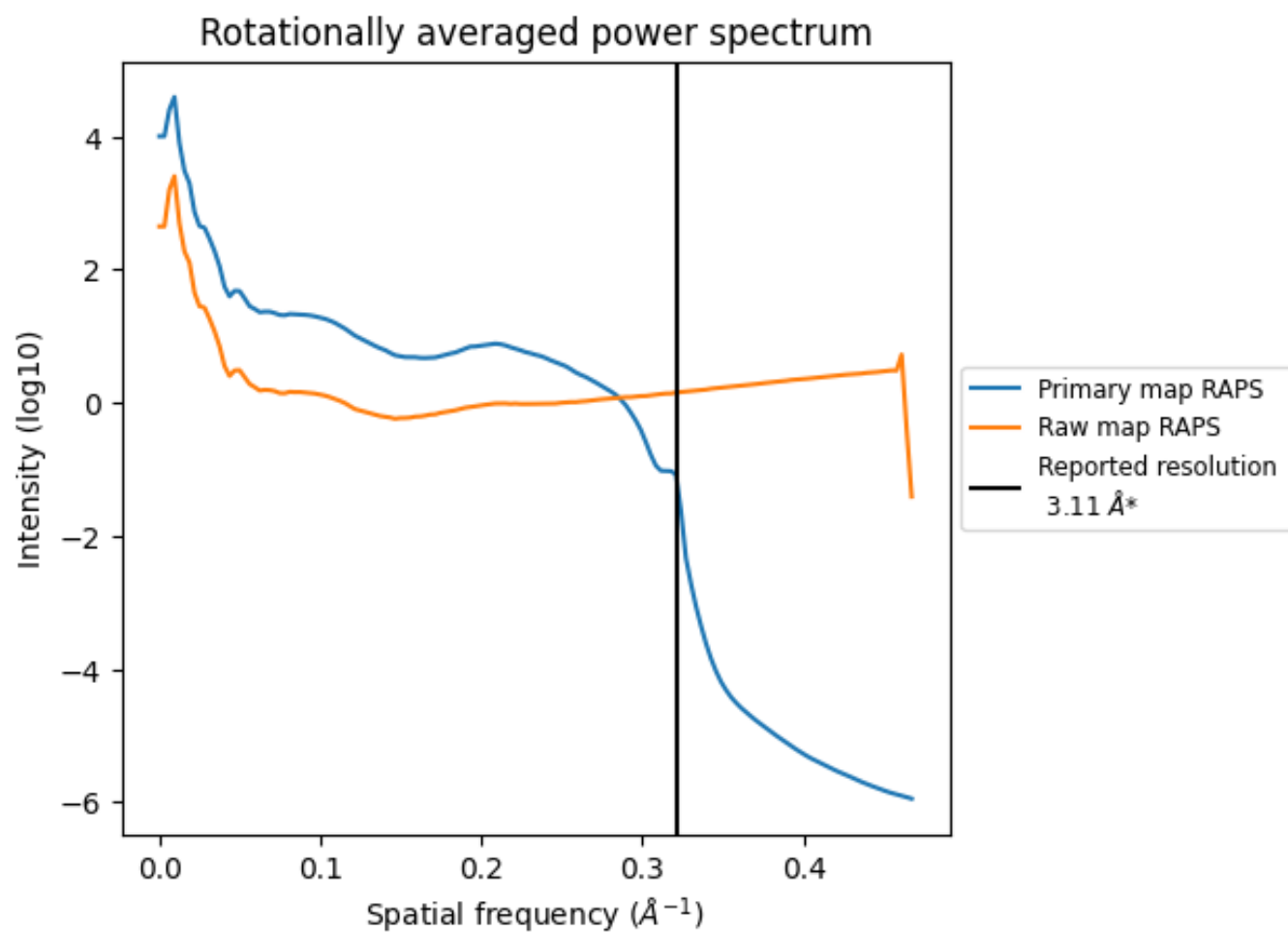
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

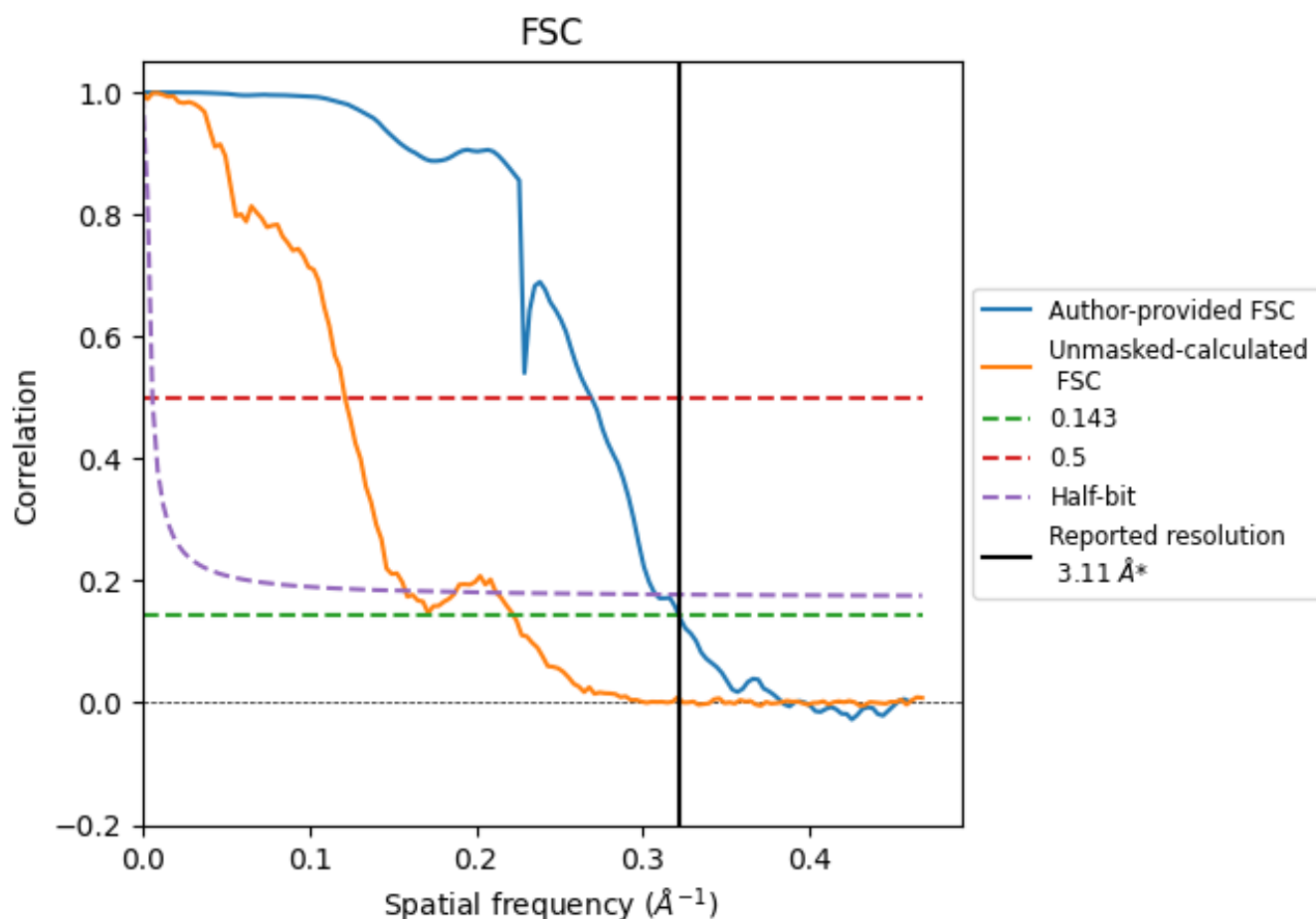


*Reported resolution corresponds to spatial frequency of $0.322 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

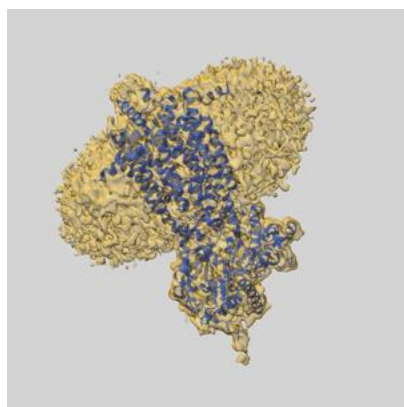
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.72	3.25
Unmasked-calculated*	4.50	8.24	6.34

*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 4.50 differs from the reported value 3.11 by more than 10 %

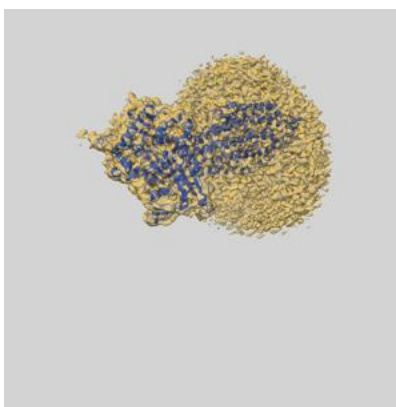
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42854 and PDB model 8V0G. Per-residue inclusion information can be found in section [3](#) on page [5](#).

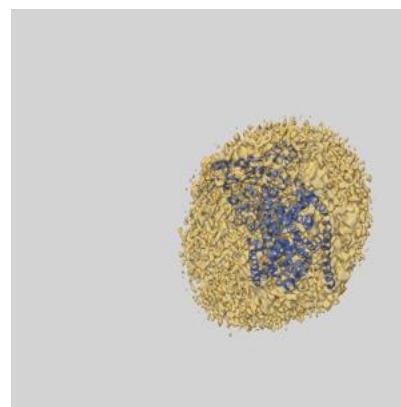
9.1 Map-model overlay [i](#)



X



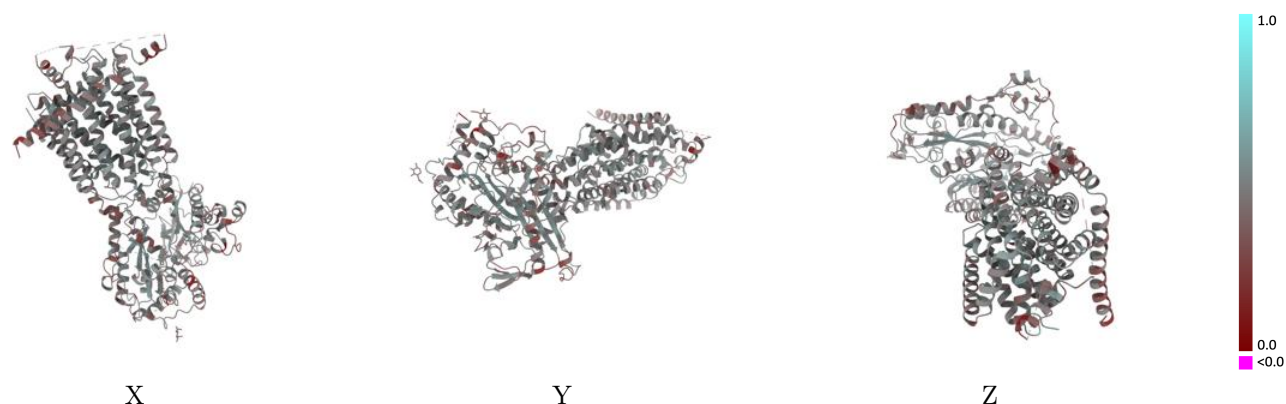
Y



Z

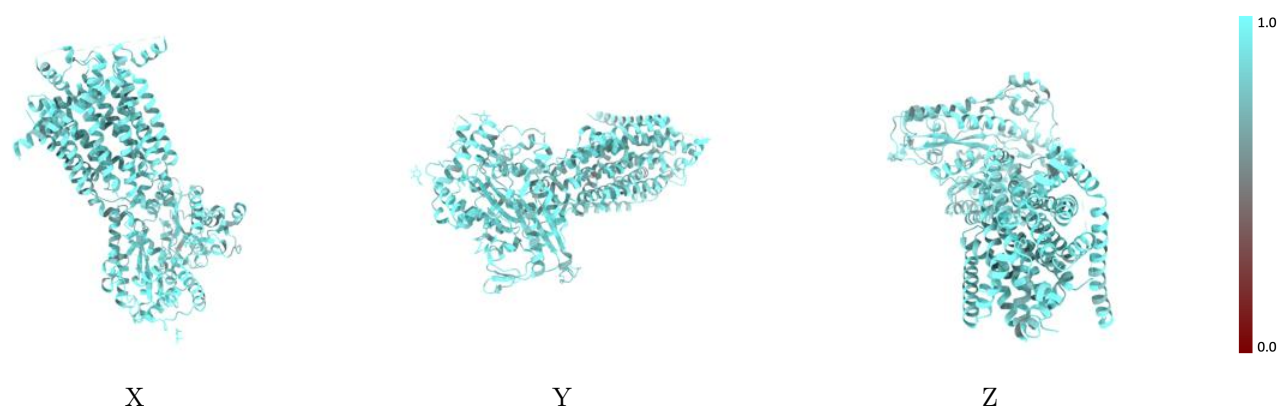
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



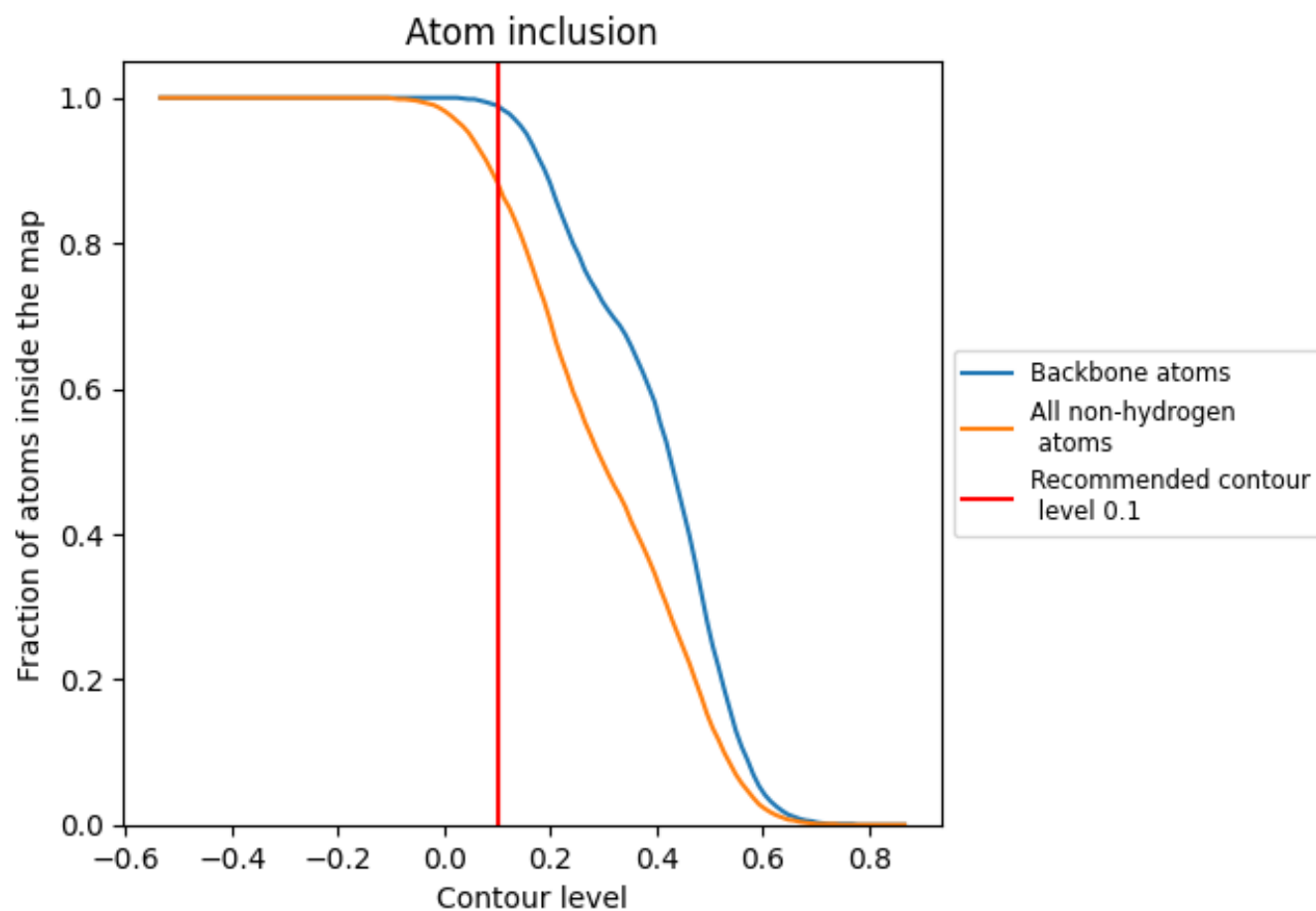
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.4580
A	0.8840	0.4580

