



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 9D30 / pdb_00009d30
EMDB ID : EMD-46506
Title : Cryo-EM structure of mycocerosic acid synthase with a single DH-ACP crosslink using C16 alpha-bromoamide. Complex C
Authors : Heberlig, G.W.; Jiang, Z.; Burkart, M.D.
Deposited on : 2024-08-09
Resolution : 3.74 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

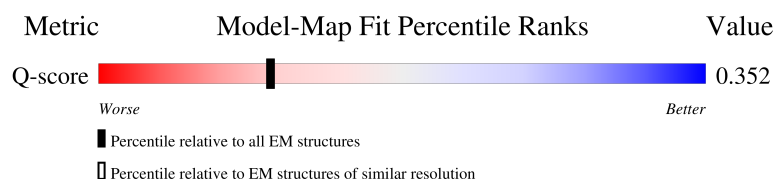
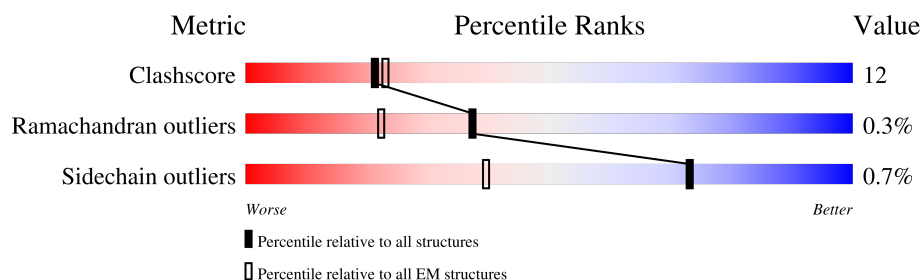
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 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	10346 (3.24 - 4.24)

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	2124	 <div>44%13%43%</div>
1	B	2124	 <div>40%12%48%</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34840 atoms, of which 17255 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.

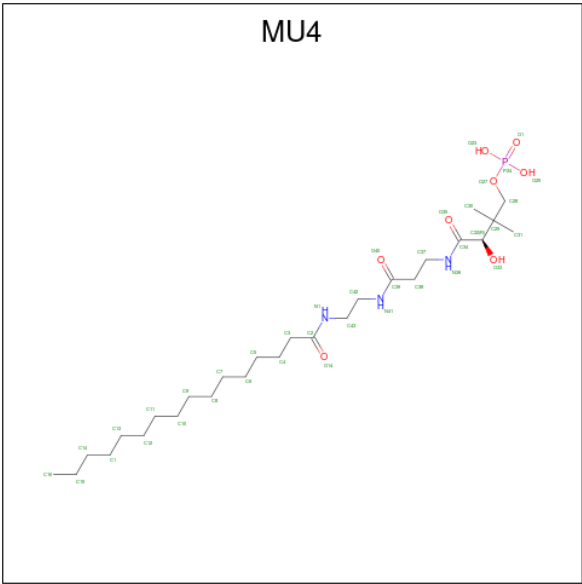
- Molecule 1 is a protein called Mycocerosic acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1215	Total	C	H	N	O	S	0	0
			18247	5745	9050	1663	1760	29		
1	B	1109	Total	C	H	N	O	S	0	0
			16567	5227	8205	1509	1601	25		

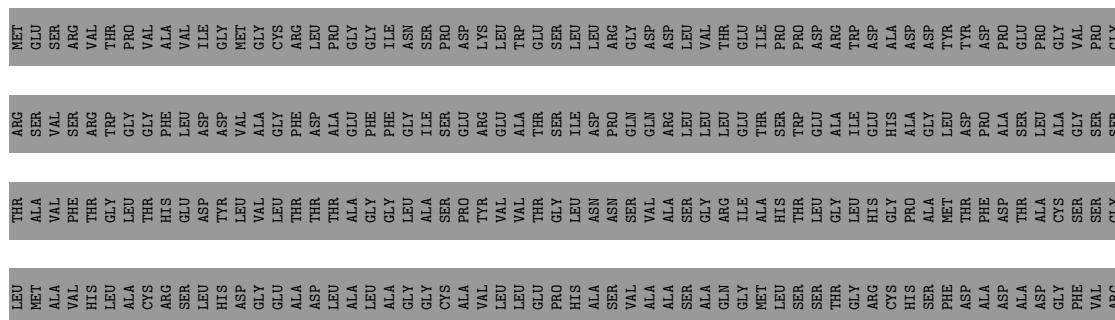
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2112	LYS	-	expression tag	UNP A0A0E8V6Y3
A	2113	LEU	-	expression tag	UNP A0A0E8V6Y3
A	2114	ALA	-	expression tag	UNP A0A0E8V6Y3
A	2115	ALA	-	expression tag	UNP A0A0E8V6Y3
A	2116	ALA	-	expression tag	UNP A0A0E8V6Y3
A	2117	LEU	-	expression tag	UNP A0A0E8V6Y3
A	2118	GLU	-	expression tag	UNP A0A0E8V6Y3
A	2119	HIS	-	expression tag	UNP A0A0E8V6Y3
A	2120	HIS	-	expression tag	UNP A0A0E8V6Y3
A	2121	HIS	-	expression tag	UNP A0A0E8V6Y3
A	2122	HIS	-	expression tag	UNP A0A0E8V6Y3
A	2123	HIS	-	expression tag	UNP A0A0E8V6Y3
A	2124	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2112	LYS	-	expression tag	UNP A0A0E8V6Y3
B	2113	LEU	-	expression tag	UNP A0A0E8V6Y3
B	2114	ALA	-	expression tag	UNP A0A0E8V6Y3
B	2115	ALA	-	expression tag	UNP A0A0E8V6Y3
B	2116	ALA	-	expression tag	UNP A0A0E8V6Y3
B	2117	LEU	-	expression tag	UNP A0A0E8V6Y3
B	2118	GLU	-	expression tag	UNP A0A0E8V6Y3
B	2119	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2120	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2121	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2122	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2123	HIS	-	expression tag	UNP A0A0E8V6Y3
B	2124	HIS	-	expression tag	UNP A0A0E8V6Y3

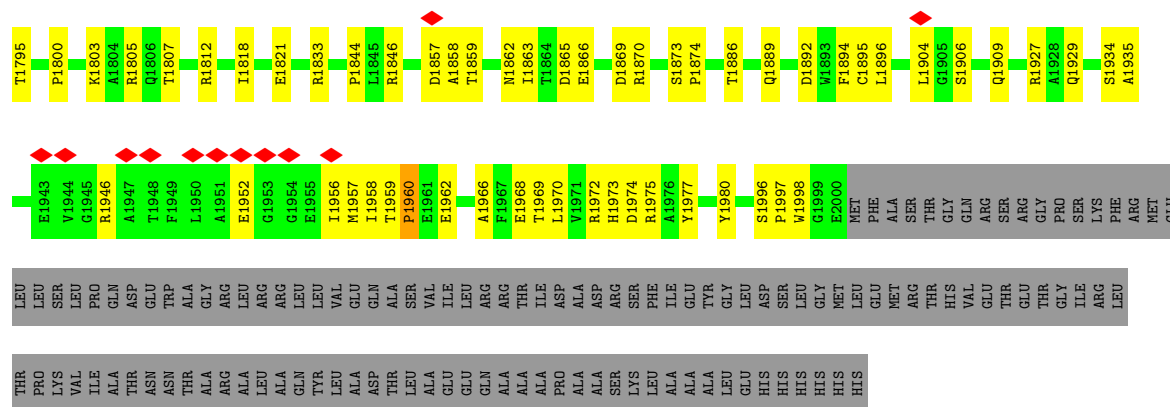
- Molecule 2 is N-[2-(hexadecanoylamino)ethyl]-N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alaninamide (CCD ID: MU4) (formula: C₂₇H₅₄N₃O₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	26	15	3	7	1	0



R1409	D1417	H1418	R1422	V1423	Q1424	D1430	L1431	Q1432	S1466	I1473	E1483	V1513	L1531	T1532	A1540	T1541	Y1548	I1566	K1561	T1568	A1590	K1595	D1609	S1610	R1611	Y1626	G1627	V1628	D1629	I1630	R1633	S1634	L1635	T1636	L1644	E1645	L1646	L1647	V1793	L1794							
R1295	R1299	H1300	L1301	V1302	R1303	R1306	E1312	L1318	F1319	V1320	V1321	Q1324	V1328	K1329	R1336	L1339	L1347	L1348	I1351	H1355	M1357	L1358	R1359	T1360	D1364	V1365	D1366	T1369	D1385	E1386	T1387	R1390	D1393	V1396	L1399	L1404	E1407	E1408									
G1173	R1184	R1189	L1190	L1191	T1192	L1193	Q1197	P1201	E1202	V1203	G1204	D1205	W1211	A1219	V1220	D1221	P1239	T1242	E1243	S1246	L1247	S1248	W1249	T1251	Q1252	D1253	T1254	P1255	P1256	N1257	A1260	L1265	R1270	V1276	I1277	V1278	Y1279	R1282	P1286	D1287							
A1063	E1064	A1065	G1066	A1067	T1068	Q1083	L1093	A1096	C1097	F1098	Q1099	G1102	A1103	Q1106	A1107	G1108	T1109	A1110	T1111	G1112	L1115	L1116	P1117	L1118	G1119	L1123	R1124	A1125	T1129	R1130	R1133	Y1134	C1135	Y1136	T1137	G1149	D1158	E1159	H1160	G1161	T1162	L1165	A1166	R1171			
D928	M945	A946	L947	A950	E959	E966	Q967	M968	L969	D972	E973	I977	I983	R997	E1000	A1008	L1009	R1010	Q1028	A1029	H1030	V1034	H1035	G1036	T1037	A1038	M1039	R1040	E1041	S1042	F1043	A1044	E1045	R1046	G1047	G1051	A1052	A1053	F1054	L1057	T1058	T1059	A1060	H1061	T1062		
LEU	THR	GLY	LEU	HIS	ARG	ALA	GLY	ALA	LEU	ASP	LEU	PRO	ALA	GLY	ASP	THR	LEU	PRO	THR	THR	HIS	ALA	LEU	ILE	ASP	ASP	GLY	GLN	GLU	GLN	ARG	ALA	PRO	ILE	ALA	ARG	GLY	THR	ASP	CYS	T892	L899	V913	W914	D917		
VAL	GLN	PHE	ALA	ALA	VAL	GLN	ALA	MET	GLU	ASP	GLY	GLY	ASP	GLY	THR	LEU	PRO	THR	THR	GLY	THR	GLY	THR	ASP	ASP	ASP	VAL	VAL	ALA	GLU	GLN	GLN	THR	VAL	VAL	THR	ASP	GLY	THR	ASP	ARG	GLY	VAL	GLY			
ALA	VAL	ASP	ALA	SER	HIS	PRO	GLN	SER	ASP	ILE	THR	ASP	ALA	ALA	ILE	VAL	ASP	VAL	VAL	GLN	SER	GLY	THR	GLY	THR	ASP	ALA	ALA	THR	ALA	VAL	ILE	CYS	THR	VAL	GLY	THR	ASP	ARG	GLY	TYR	TRP	VAL	ASP	THR		
GLY	SER	TRP	ALA	ALA	THR	MET	THR	GLY	LEU	VAL	PHE	ALA	ALA	ALA	ILE	VAL	GLY	VAL	VAL	GLN	SER	GLY	THR	GLY	THR	GLY	ALA	ALA	THR	ALA	GLN	THR	VAL	GLY	THR	ASP	ILE	ASP	ARG	GLY	PRO	GLY	THR	VAL	GLN		
ASN	VAL	HIS	VAL	VAL	GLY	ALA	GLY	ALA	SER	PRO	GLY	VAL	VAL	VAL	PRO	GLY	VAL	VAL	VAL	GLY	SER	GLY	THR	GLY	THR	ASP	ALA	ALA	THR	ALA	ARG	GLN	THR	VAL	VAL	GLY	THR	ASP	ARG	GLY	TYR	VAL	VAL	GLY	THR	ALA	
ALA	ILE	LEU	SER	ALA	THR	THR	THR	LEU	SER	THR	THR	PRO	ASP	GLY	ASP	THR	GLY	THR	THR	PRO	GLN	GLY	THR	THR	THR	ASP	ALA	ALA	THR	ALA	ARG	GLN	THR	VAL	VAL	GLY	THR	ASP	ARG	GLY	TYR	VAL	VAL	GLY	THR	ALA	
VAL	GLN	PRO	GLY	THR	VAL	GLY	HIS	GLY	THR	THR	THR	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35969	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.267	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	341.376, 341.376, 341.376	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.889, 0.889, 0.889	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MU4

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	0.20	0/9380	0.38	4/12768 (0.0%)
1	B	0.14	0/8534	0.31	1/11626 (0.0%)
All	All	0.18	0/17914	0.35	5/24394 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2061	LEU	N-CA-C	-7.82	103.70	113.55
1	B	1960	PRO	CA-N-CD	-6.77	102.52	112.00
1	A	2062	GLY	N-CA-C	-6.31	104.92	113.37
1	A	2060	SER	N-CA-C	-6.15	106.19	113.38
1	A	926	LEU	N-CA-C	-5.39	104.81	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1189	ARG	Sidechain
1	A	2045	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9197	9050	9053	229	0
1	B	8362	8205	8206	189	0
2	A	26	0	0	8	0
All	All	17585	17255	17259	411	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 12.

All (411) 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:1116:LEU:HD21	2:A:2201:MU4:C38	1.93	0.99
1:A:1095:ASP:OD1	2:A:2201:MU4:C5	2.12	0.97
1:A:2035:LEU:HD21	1:A:2092:LEU:HD22	1.50	0.92
1:A:1636:THR:OG1	1:A:1660:ASP:OD1	1.95	0.83
1:A:1070:VAL:O	1:A:1134:TYR:OH	1.96	0.82
1:A:1215:ASP:OD1	1:A:1218:ASN:ND2	2.13	0.81
1:A:1287:ASP:OD1	1:A:1288:GLU:N	2.13	0.80
1:B:1028:GLN:NE2	1:B:1064:GLU:OE2	2.15	0.80
1:A:931:VAL:HG11	1:A:968:MET:HE1	1.65	0.79
1:B:1748:ARG:NH2	1:B:1750:SER:OG	2.15	0.78
1:A:1970:LEU:HD21	1:A:1978:SER:OG	1.84	0.77
1:A:947:LEU:HD21	1:A:1123:LEU:HD22	1.67	0.76
1:A:1459:ASN:OD1	1:A:1738:LYS:NZ	2.18	0.76
1:A:1909:GLN:N	1:A:1909:GLN:OE1	2.18	0.76
1:A:1299:ARG:NE	1:A:1865:ASP:OD2	2.18	0.76
1:A:1202:GLU:O	1:A:1204:GLY:N	2.20	0.75
1:A:1061:HIS:O	1:A:1071:LEU:N	2.20	0.74
1:B:1306:ARG:NH2	1:B:1863:ILE:O	2.19	0.74
1:B:1540:ALA:O	1:B:1541:THR:OG1	2.02	0.74
1:A:1089:ILE:HD13	1:A:1165:LEU:HD12	1.69	0.73
1:A:1364:ASP:OD2	1:A:1390:ARG:NH2	2.21	0.73
1:A:1225:MET:HE3	1:A:1225:MET:H	1.54	0.73
1:A:929:HIS:CE1	2:A:2201:MU4:N1	2.48	0.73
1:A:1408:GLU:N	1:A:1408:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1359:ARG:NH2	1:B:1385:ASP:OD1	2.23	0.72
1:A:1329:LYS:O	1:A:1333:SER:OG	2.05	0.72
1:B:959:GLU:N	1:B:959:GLU:OE1	2.23	0.72
1:B:1456:SER:HG	1:B:1513:TRP:CD1	2.08	0.71
1:B:1846:ARG:NE	1:B:1892:ASP:OD1	2.24	0.71
1:B:1927:ARG:NH1	1:B:1974:ASP:OD1	2.24	0.70
1:A:1377:GLN:OE1	1:A:1394:TRP:NE1	2.25	0.69
1:A:1424:GLN:O	1:A:1424:GLN:NE2	2.25	0.69
1:A:1123:LEU:HD23	1:A:1124:ARG:N	2.06	0.69
1:B:1959:THR:HG22	1:B:1962:GLU:HB2	1.75	0.68
1:B:1366:ASP:OD2	1:B:1390:ARG:NE	2.28	0.67
1:A:1211:TRP:O	1:A:1272:ARG:NH1	2.26	0.67
1:A:1225:MET:SD	1:A:1226:LEU:N	2.67	0.67
1:B:1548:TYR:OH	1:B:1693:ARG:NH1	2.28	0.67
1:B:1690:GLN:OE1	1:B:1693:ARG:NE	2.28	0.66
1:A:1409:ARG:NH2	1:A:1435:GLU:OE2	2.28	0.66
1:B:1276:VAL:HG22	1:B:1319:PHE:HB2	1.77	0.66
1:A:1899:SER:N	1:A:1916:ASN:OD1	2.28	0.66
1:B:1609:ASP:OD1	1:B:1611:ARG:N	2.29	0.66
1:A:1358:LEU:HD12	1:A:1358:LEU:O	1.97	0.64
1:A:1685:LEU:O	1:A:1689:THR:HG22	1.96	0.64
1:A:1812:ARG:NH1	1:A:1818:ILE:O	2.30	0.64
1:A:1956:ILE:HG23	1:A:1957:MET:HG3	1.80	0.64
1:B:1197:GLN:NE2	1:B:1393:ASP:OD2	2.31	0.64
1:A:1768:ILE:CG2	1:A:1848:VAL:HG22	2.28	0.63
1:B:1644:LEU:HD22	1:B:1667:LEU:HD11	1.80	0.63
1:B:947:LEU:HD12	1:B:1123:LEU:HD22	1.81	0.63
1:B:1295:ARG:NH2	1:B:1869:ASP:OD1	2.32	0.62
1:B:1609:ASP:OD1	1:B:1610:SER:N	2.31	0.62
1:A:968:MET:HE2	1:A:2064:LEU:HD21	1.81	0.62
1:A:1981:ILE:HD12	1:A:1981:ILE:O	1.99	0.62
1:B:1115:LEU:HA	1:B:1172:MET:HE1	1.81	0.62
1:B:1404:LEU:HD13	1:B:1973:HIS:CE1	2.35	0.62
1:B:1757:GLN:O	1:B:1757:GLN:NE2	2.31	0.62
1:B:928:ASP:OD1	1:B:928:ASP:N	2.33	0.62
2:A:2201:MU4:C5	2:A:2201:MU4:N1	2.63	0.61
1:B:1046:ARG:NH2	1:B:1099:GLN:OE1	2.34	0.61
1:B:1866:GLU:OE1	1:B:1870:ARG:NH1	2.32	0.61
1:A:1872:TRP:CE2	1:A:1876:VAL:HG21	2.36	0.61
1:B:1417:ASP:OD1	1:B:1418:HIS:N	2.33	0.61
1:A:1221:ASP:OD1	1:A:1222:THR:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1958:ILE:O	1:A:1959:THR:OG1	2.13	0.61
1:B:983:ILE:HG23	1:B:983:ILE:O	2.00	0.60
1:B:1886:THR:O	1:B:1889:GLN:NE2	2.34	0.60
1:A:1939:GLY:HA3	1:A:1981:ILE:HG22	1.84	0.60
1:B:1083:GLN:N	1:B:1083:GLN:OE1	2.35	0.60
1:A:908:GLU:OE2	1:B:1665:THR:OG1	2.14	0.60
1:A:1629:ASP:C	1:A:1630:ILE:HD12	2.27	0.59
1:B:1299:ARG:NH2	1:B:1869:ASP:OD1	2.33	0.59
1:A:1276:VAL:HG23	1:A:1319:PHE:HB3	1.83	0.59
1:A:1374:VAL:O	1:A:1378:LEU:HD23	2.02	0.59
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.35	0.59
1:B:1249:TRP:CD1	1:B:1254:THR:HG1	2.20	0.59
1:B:1531:LEU:O	1:B:1532:THR:OG1	2.15	0.59
1:A:1098:PHE:O	1:A:1101:VAL:HG12	2.03	0.59
1:B:1158:ASP:OD1	1:B:1162:THR:N	2.35	0.59
1:A:1028:GLN:N	1:A:1028:GLN:OE1	2.36	0.58
1:B:968:MET:SD	1:B:969:LEU:N	2.77	0.58
1:B:1149:GLY:O	1:B:1173:GLY:N	2.36	0.58
1:A:938:PRO:HA	2:A:2201:MU4:C43	2.34	0.58
1:A:991:PHE:HB2	1:A:1009:LEU:HD11	1.86	0.58
1:B:1251:VAL:O	1:B:1252:GLN:NE2	2.37	0.58
1:A:932:HIS:NE2	1:A:2065:GLU:OE1	2.37	0.58
1:A:1339:LEU:HD23	1:A:1918:TRP:CZ2	2.39	0.58
1:A:1667:LEU:HD12	1:A:1667:LEU:O	2.04	0.58
1:A:1253:ASP:OD2	1:A:1257:ASN:ND2	2.36	0.57
1:B:1929:GLN:O	1:B:1929:GLN:NE2	2.37	0.57
1:A:1689:THR:HG21	1:B:1649:PHE:CE2	2.39	0.57
1:A:905:LEU:CD2	1:B:913:VAL:HG21	2.35	0.57
1:A:1364:ASP:OD1	1:A:1365:VAL:N	2.37	0.57
1:A:2016:ARG:NH1	1:A:2016:ARG:O	2.37	0.57
1:B:1568:THR:HG21	1:B:1595:LYS:HD2	1.85	0.57
1:A:1661:VAL:HG21	1:A:1680:TYR:CE1	2.39	0.57
1:B:1062:THR:OG1	1:B:1069:THR:HG23	2.05	0.57
1:B:1324:GLN:N	1:B:1365:VAL:O	2.38	0.56
1:B:1626:TYR:O	1:B:1648:ALA:HB2	2.05	0.56
1:A:1136:TYR:O	1:A:1154:LEU:HD23	2.05	0.56
1:A:1794:LEU:HD23	1:A:1795:THR:N	2.21	0.56
1:A:2060:SER:HA	1:A:2063:MET:HB2	1.85	0.56
1:A:1165:LEU:HD23	1:A:1166:ALA:N	2.21	0.56
1:B:947:LEU:HD12	1:B:1123:LEU:CD2	2.36	0.56
1:B:1328:VAL:HG22	1:B:1329:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:GLU:N	1:B:1493:GLU:OE1	2.36	0.56
1:A:1030:HIS:O	1:A:1071:LEU:HD12	2.05	0.56
1:A:1764:ASP:OD1	1:A:1846:ARG:NH2	2.34	0.56
1:B:1647:LEU:HD12	1:B:1651:GLY:HA3	1.88	0.56
1:B:1286:PRO:HB3	1:B:1339:LEU:HD13	1.87	0.56
1:A:1088:ARG:O	1:A:1089:ILE:HD12	2.06	0.55
1:B:1034:VAL:HA	1:B:1059:THR:HG23	1.87	0.55
1:B:1904:LEU:C	1:B:1904:LEU:HD23	2.30	0.55
1:A:1846:ARG:C	1:A:1891:LEU:HD12	2.30	0.55
1:B:1093:LEU:CD2	1:B:1129:THR:HG21	2.37	0.55
1:B:1243:GLU:OE1	1:B:1243:GLU:N	2.39	0.55
1:A:1763:ARG:NH2	1:A:1787:ALA:O	2.37	0.55
1:B:1318:LEU:HD23	1:B:1358:LEU:HD13	1.87	0.55
1:B:1946:ARG:NH1	1:B:1952:GLU:O	2.40	0.55
1:B:1158:ASP:OD1	1:B:1161:GLY:N	2.38	0.55
1:A:1499:GLN:N	1:A:1499:GLN:OE1	2.38	0.55
1:A:1172:MET:SD	1:A:1172:MET:N	2.80	0.54
1:B:1760:LEU:HD12	1:B:1761:TYR:CD1	2.41	0.54
1:B:917:ASP:OD1	1:B:917:ASP:C	2.50	0.54
1:A:1046:ARG:NH1	1:A:1113:GLY:O	2.36	0.54
1:A:1669:LEU:HD21	1:B:1661:VAL:HG22	1.90	0.54
1:B:1969:THR:O	1:B:1973:HIS:ND1	2.38	0.54
1:B:1066:GLY:O	1:B:1069:THR:HG22	2.07	0.54
1:B:1312:GLU:OE1	1:B:1312:GLU:N	2.38	0.54
1:A:1000:GLU:N	1:A:1000:GLU:OE1	2.41	0.54
1:A:1083:GLN:OE1	1:A:1083:GLN:N	2.41	0.54
1:A:1872:TRP:CD2	1:A:1876:VAL:HG21	2.43	0.54
1:B:1771:GLY:N	1:B:1795:THR:O	2.39	0.54
1:A:1088:ARG:C	1:A:1089:ILE:HD12	2.33	0.54
1:B:1407:GLU:N	1:B:1407:GLU:OE1	2.40	0.54
1:B:1422:ARG:NH1	1:B:1424:GLN:OE1	2.38	0.54
1:B:1432:GLN:OE1	1:B:1728:ARG:NH2	2.41	0.53
1:A:1404:LEU:HD13	1:A:1973:HIS:CG	2.44	0.53
1:B:1866:GLU:OE2	1:B:1870:ARG:NH2	2.41	0.53
1:A:2078:LEU:HD23	1:A:2078:LEU:H	1.73	0.53
1:A:1613:VAL:HG12	1:A:1613:VAL:O	2.08	0.53
1:B:1037:THR:O	1:B:1041:GLU:N	2.31	0.53
1:A:1326:GLN:O	1:A:1390:ARG:NH2	2.38	0.53
1:B:1859:THR:O	1:B:1862:ASN:N	2.39	0.53
1:A:1725:ASP:OD1	1:A:1726:ALA:N	2.42	0.53
1:A:1048:VAL:HG13	1:A:1048:VAL:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1756:GLU:N	1:A:1756:GLU:OE1	2.42	0.53
1:A:912:HIS:CE1	1:A:953:VAL:HG23	2.44	0.52
1:A:1437:VAL:HG13	1:A:1755:PRO:HD3	1.92	0.52
1:A:1301:LEU:HD12	1:A:1301:LEU:O	2.09	0.52
1:A:1669:LEU:HD23	1:B:1661:VAL:HG13	1.92	0.52
1:B:1956:ILE:HG23	1:B:1957:MET:SD	2.50	0.52
1:B:1043:PHE:O	1:B:1047:GLY:N	2.37	0.52
1:B:1404:LEU:HD22	1:B:1973:HIS:CD2	2.45	0.52
1:A:1372:GLU:N	1:A:1372:GLU:OE1	2.42	0.52
1:A:1123:LEU:HG	1:A:1167:VAL:HG12	1.90	0.52
1:A:1629:ASP:HB3	1:A:1630:ILE:HD12	1.93	0.51
1:A:1791:ARG:HE	1:A:1841:THR:HG21	1.74	0.51
1:A:1900:GLY:N	1:A:1938:TRP:O	2.42	0.51
1:A:1223:PRO:HA	1:A:1225:MET:HE1	1.92	0.51
1:B:1399:LEU:HD22	1:B:1998:TRP:HE3	1.75	0.51
1:A:1540:ALA:O	1:A:1541:THR:OG1	2.17	0.51
1:B:1008:ALA:HB1	1:B:1010:ARG:HH12	1.76	0.51
1:A:1327:ILE:HD11	1:A:1334:GLY:N	2.26	0.51
1:B:1278:VAL:HG12	1:B:1321:VAL:HB	1.93	0.51
1:A:1689:THR:HG21	1:B:1649:PHE:CD2	2.46	0.51
1:A:1474:ASP:O	1:A:1475:ASP:OD1	2.28	0.51
1:B:1251:VAL:HG23	1:B:1252:GLN:HE21	1.76	0.51
1:B:1255:PRO:N	1:B:1256:PRO:HD2	2.26	0.51
1:B:1959:THR:N	1:B:1960:PRO:HD2	2.26	0.51
1:B:1062:THR:HG1	1:B:1069:THR:HG23	1.75	0.50
1:A:929:HIS:CE1	2:A:2201:MU4:C43	2.94	0.50
1:B:1556:ILE:CD1	1:B:1630:ILE:HD13	2.40	0.50
1:A:1568:THR:HG21	1:A:1595:LYS:HB3	1.92	0.50
1:A:1916:ASN:O	1:A:1919:VAL:HG12	2.12	0.50
1:B:1645:GLU:OE1	1:B:1645:GLU:C	2.54	0.50
1:A:1939:GLY:CA	1:A:1981:ILE:HG22	2.41	0.50
1:B:1649:PHE:CD1	1:B:1649:PHE:C	2.88	0.50
1:A:1431:LEU:HD11	1:A:1728:ARG:NH2	2.27	0.50
1:A:1791:ARG:HH12	1:A:1819:VAL:HG11	1.76	0.50
1:B:950:ALA:HB2	1:B:1009:LEU:HD22	1.93	0.50
1:A:1386:GLU:HG3	1:A:1397:ALA:HB3	1.92	0.50
1:B:1135:CYS:SG	1:B:1137:THR:HG23	2.51	0.50
1:B:1254:THR:N	1:B:1255:PRO:CD	2.75	0.50
1:B:1548:TYR:HB2	1:B:1697:LEU:HD11	1.94	0.50
1:A:1768:ILE:HG22	1:A:1848:VAL:HG22	1.94	0.49
1:A:1147:THR:O	1:A:1148:ARG:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:LEU:C	1:A:1431:LEU:HD12	2.37	0.49
1:B:1328:VAL:HG13	1:B:1329:LYS:O	2.11	0.49
1:B:1112:GLY:O	1:B:1184:ARG:NH2	2.46	0.49
1:A:908:GLU:OE1	1:A:908:GLU:N	2.39	0.49
1:A:983:ILE:HG22	1:A:983:ILE:O	2.11	0.49
1:A:1190:LEU:O	1:A:1191:LEU:HD23	2.13	0.49
1:A:1285:ASP:OD1	1:A:1285:ASP:N	2.46	0.49
1:A:1202:GLU:O	1:A:1203:VAL:HG12	2.12	0.49
1:A:1351:ILE:HD12	1:A:1860:LEU:CD1	2.42	0.49
1:B:947:LEU:HD11	1:B:1125:ALA:HB3	1.94	0.49
1:B:1172:MET:HE3	1:B:1172:MET:O	2.13	0.49
1:B:1133:ARG:HG3	1:B:1159:GLU:HG2	1.95	0.48
1:B:1431:LEU:HD22	1:B:1728:ARG:HD2	1.94	0.48
1:B:1669:LEU:HD23	1:B:1669:LEU:C	2.38	0.48
1:A:1232:ASP:C	1:A:1232:ASP:OD1	2.56	0.48
1:B:1347:LEU:O	1:B:1351:ILE:HG12	2.14	0.48
1:B:1365:VAL:HG12	1:B:1366:ASP:N	2.27	0.48
1:A:1386:GLU:CG	1:A:1397:ALA:HB3	2.44	0.48
1:A:2035:LEU:CD2	1:A:2092:LEU:HD22	2.31	0.48
1:B:1628:VAL:HG12	1:B:1629:ASP:H	1.79	0.48
1:A:1191:LEU:HD11	1:A:1981:ILE:HD11	1.96	0.48
1:A:1983:ILE:HG13	1:A:1984:LEU:H	1.78	0.48
1:B:899:LEU:HD13	1:B:914:TRP:CE3	2.48	0.48
1:B:1165:LEU:HD12	1:B:1166:ALA:N	2.29	0.48
1:B:1189:ARG:O	1:B:1191:LEU:HD12	2.14	0.48
1:B:1456:SER:HG	1:B:1513:TRP:HD1	1.57	0.48
1:B:1682:ASP:OD1	1:B:1682:ASP:C	2.57	0.47
1:A:929:HIS:HE1	2:A:2201:MU4:C43	2.27	0.47
1:A:930:GLN:HA	1:A:934:VAL:O	2.13	0.47
1:A:1609:ASP:OD1	1:A:1610:SER:N	2.46	0.47
1:B:1054:PHE:CD2	1:B:1057:LEU:HD12	2.48	0.47
1:A:1459:ASN:N	1:A:1462:ASP:OD2	2.48	0.47
1:A:2025:ASP:N	1:A:2025:ASP:OD1	2.47	0.47
1:A:1423:VAL:HG21	1:A:1720:LEU:HD21	1.97	0.47
1:B:1279:TYR:OH	1:B:1301:LEU:HD11	2.15	0.47
1:B:1792:ILE:HD13	1:B:1818:ILE:HG22	1.96	0.47
1:A:1191:LEU:CD1	1:A:1981:ILE:HD11	2.45	0.47
1:A:1431:LEU:HD11	1:A:1728:ARG:HH21	1.80	0.47
1:A:1791:ARG:NH1	1:A:1819:VAL:HG11	2.29	0.47
1:A:1893:TRP:CD1	1:A:1893:TRP:C	2.92	0.47
1:B:1633:ASN:OD1	1:B:1634:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1661:VAL:HG21	1:B:1680:TYR:CE2	2.49	0.47
1:B:1766:SER:N	1:B:1844:PRO:O	2.45	0.47
1:A:910:GLU:OE1	1:A:910:GLU:HA	2.15	0.47
1:B:1404:LEU:HD13	1:B:1973:HIS:NE2	2.30	0.47
1:A:1399:LEU:O	1:A:1399:LEU:HD23	2.14	0.47
1:A:1628:VAL:HG12	1:A:1646:LEU:HD22	1.97	0.47
1:A:1901:ALA:O	1:A:1905:GLY:N	2.48	0.47
1:A:931:VAL:HG13	1:A:931:VAL:O	2.15	0.47
1:A:1098:PHE:O	1:A:1100:SER:N	2.48	0.47
1:A:2022:LEU:HD12	1:A:2022:LEU:H	1.80	0.47
1:B:1093:LEU:HD22	1:B:1129:THR:HG21	1.96	0.46
1:B:1904:LEU:HD22	1:B:1906:SER:HB2	1.96	0.46
1:A:966:GLU:N	1:A:1004:HIS:O	2.49	0.46
1:B:1065:ALA:HB3	1:B:1069:THR:HG21	1.97	0.46
1:A:970:LEU:HD22	1:A:2077:ARG:CD	2.45	0.46
1:A:1636:THR:OG1	1:A:1637:GLY:N	2.49	0.46
1:A:1920:ASP:OD2	1:A:1977:TYR:CZ	2.69	0.46
1:B:1754:THR:HG21	1:B:1758:ALA:HB2	1.98	0.46
1:A:2019:LEU:O	1:A:2022:LEU:HD12	2.16	0.46
1:B:1720:LEU:HD22	1:B:1743:VAL:HG22	1.97	0.46
1:B:1812:ARG:NH2	1:B:1818:ILE:O	2.49	0.46
1:B:1399:LEU:HD22	1:B:1998:TRP:CE3	2.50	0.46
1:B:1430:ASP:OD1	1:B:1432:GLN:N	2.49	0.46
1:A:1956:ILE:C	1:A:1957:MET:HG3	2.41	0.46
1:B:1251:VAL:HG12	1:B:1300:HIS:CD2	2.51	0.46
1:B:1647:LEU:HD21	1:B:1676:LEU:CD2	2.46	0.46
1:A:1191:LEU:N	1:A:1979:GLY:O	2.49	0.45
1:B:1365:VAL:HG12	1:B:1366:ASP:H	1.80	0.45
1:A:1459:ASN:O	1:A:1462:ASP:N	2.49	0.45
1:A:1234:LEU:HD12	1:A:1379:LEU:HD21	1.96	0.45
1:B:1727:ILE:O	1:B:1728:ARG:C	2.59	0.45
1:A:1269:LEU:N	1:A:1269:LEU:HD23	2.32	0.45
1:A:1457:SER:HB3	1:A:1537:ILE:HD11	1.99	0.45
1:A:1860:LEU:HA	1:A:1863:ILE:HD12	1.99	0.45
1:A:1097:CYS:O	1:A:1154:LEU:HD11	2.16	0.45
1:A:1667:LEU:HD12	1:A:1667:LEU:C	2.41	0.45
1:B:1030:HIS:ND1	1:B:1062:THR:HG23	2.31	0.45
1:A:970:LEU:HD22	1:A:2077:ARG:HD3	1.98	0.45
1:A:1123:LEU:HD23	1:A:1124:ARG:H	1.79	0.45
1:A:1275:VAL:HG11	1:A:1308:LEU:HD21	1.98	0.45
1:A:1655:GLU:OE2	1:A:1655:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2012:PRO:O	1:A:2014:LYS:N	2.50	0.45
1:B:1036:GLY:O	1:B:1039:MET:HE3	2.17	0.45
1:A:1439:SER:O	1:A:1440:ASP:OD1	2.35	0.45
1:A:927:SER:O	1:A:928:ASP:CG	2.60	0.44
1:A:1220:VAL:HG12	1:A:1221:ASP:N	2.31	0.44
1:A:1416:PRO:HG3	1:A:1421:MET:HE1	1.99	0.44
1:B:1760:LEU:HD12	1:B:1761:TYR:HD1	1.80	0.44
1:A:1471:PRO:O	1:A:1473:ILE:HG23	2.17	0.44
1:B:1895:CYS:SG	1:B:1934:SER:OG	2.74	0.44
1:A:899:LEU:HD21	1:A:945:MET:HG3	1.99	0.44
1:B:1896:LEU:N	1:B:1896:LEU:HD22	2.33	0.44
1:B:1287:ASP:O	1:B:1290:SER:OG	2.35	0.44
1:A:1263:GLU:O	1:A:1267:SER:OG	2.24	0.44
1:B:1357:MET:C	1:B:1357:MET:SD	3.01	0.44
1:B:1548:TYR:CD2	1:B:1686:MET:HE1	2.53	0.44
1:B:1057:LEU:HD21	1:B:1096:ALA:O	2.18	0.44
1:A:1462:ASP:OD1	1:A:1481:GLY:N	2.49	0.44
1:B:947:LEU:HD11	1:B:1125:ALA:CB	2.47	0.44
1:A:970:LEU:HB2	1:A:2077:ARG:NH2	2.33	0.43
1:A:1507:PHE:CZ	1:A:1698:LEU:HD11	2.53	0.43
1:A:1808:ILE:HG23	1:A:1818:ILE:HD11	1.99	0.43
1:A:2078:LEU:HD23	1:A:2078:LEU:N	2.33	0.43
1:B:1540:ALA:C	1:B:1541:THR:HG1	2.11	0.43
1:B:1655:GLU:OE2	1:B:1655:GLU:HA	2.18	0.43
1:B:1904:LEU:HD23	1:B:1904:LEU:O	2.17	0.43
1:A:1129:THR:CG2	1:A:1132:ALA:HB2	2.47	0.43
1:B:1037:THR:O	1:B:1040:ARG:N	2.46	0.43
1:A:1080:ILE:O	1:A:1080:ILE:HG22	2.18	0.43
1:A:1164:LEU:N	1:A:1164:LEU:HD22	2.33	0.43
1:A:1269:LEU:HD23	1:A:1269:LEU:H	1.83	0.43
1:A:1751:VAL:HG23	1:A:1751:VAL:O	2.16	0.43
1:B:1358:LEU:O	1:B:1358:LEU:HD12	2.18	0.43
1:B:1821:GLU:OE2	1:B:1833:ARG:NH2	2.41	0.43
1:B:1958:ILE:O	1:B:1958:ILE:HG13	2.18	0.43
1:A:1351:ILE:HD12	1:A:1860:LEU:HD12	1.99	0.43
1:A:908:GLU:OE2	1:B:1665:THR:CB	2.67	0.43
1:A:1165:LEU:HD23	1:A:1165:LEU:C	2.43	0.43
1:A:1441:ARG:NH2	1:A:1450:GLU:OE2	2.49	0.43
1:A:1998:TRP:O	1:A:1999:GLY:C	2.61	0.43
1:A:930:GLN:HB3	1:A:933:ASN:HA	2.00	0.43
1:A:1670:PHE:N	1:A:1671:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1886:THR:HG22	1:A:1886:THR:O	2.18	0.43
1:B:1351:ILE:HD13	1:B:1351:ILE:N	2.34	0.43
1:B:1760:LEU:HD11	1:B:1968:GLU:OE2	2.19	0.43
1:B:1894:PHE:O	1:B:1934:SER:N	2.44	0.43
1:A:1301:LEU:HD23	1:A:1344:LEU:HD22	2.00	0.43
1:B:1633:ASN:OD1	1:B:1633:ASN:C	2.61	0.43
1:B:1757:GLN:O	1:B:1757:GLN:CG	2.66	0.43
1:A:1371:VAL:O	1:A:1371:VAL:HG22	2.18	0.43
1:A:1421:MET:HE3	1:A:1515:THR:HG21	2.01	0.43
1:A:1628:VAL:CG1	1:A:1646:LEU:HD22	2.49	0.43
1:A:1734:GLU:OE1	1:A:1734:GLU:N	2.48	0.43
1:B:1966:ALA:HB2	1:B:1980:TYR:CZ	2.54	0.43
1:A:1393:ASP:OD1	1:A:1394:TRP:N	2.52	0.42
1:A:1838:ALA:O	1:A:1841:THR:HG22	2.18	0.42
1:A:1927:ARG:NH2	1:A:1974:ASP:OD2	2.52	0.42
1:B:1387:THR:HG22	1:B:1396:VAL:HG22	2.01	0.42
1:B:1779:PHE:HD1	1:B:1779:PHE:O	2.01	0.42
1:A:1058:THR:HG22	1:A:1059:THR:N	2.34	0.42
1:A:1076:LEU:N	1:A:1076:LEU:HD12	2.33	0.42
1:B:1355:HIS:HB3	1:B:1358:LEU:HD21	2.00	0.42
1:B:1757:GLN:O	1:B:1757:GLN:HG2	2.19	0.42
1:B:1761:TYR:OH	1:B:1784:LEU:HD22	2.19	0.42
1:B:1286:PRO:CB	1:B:1339:LEU:HD13	2.49	0.42
1:B:1561:LYS:O	1:B:1628:VAL:HG12	2.19	0.42
1:A:1255:PRO:N	1:A:1256:PRO:HD2	2.34	0.42
1:A:1669:LEU:HD23	1:A:1669:LEU:O	2.20	0.42
1:B:997:ARG:O	1:B:1000:GLU:N	2.41	0.42
1:B:1193:LEU:HD12	1:B:1193:LEU:C	2.43	0.42
1:A:1062:THR:OG1	1:A:1069:THR:OG1	2.31	0.42
1:A:2040:SER:O	1:A:2044:ARG:N	2.49	0.42
1:B:1119:GLY:O	1:B:1171:ARG:N	2.45	0.42
1:B:1366:ASP:O	1:B:1369:THR:OG1	2.34	0.42
1:A:970:LEU:HD11	1:A:997:ARG:NH2	2.34	0.42
1:A:1274:GLY:HA2	1:A:1316:PRO:HB2	2.01	0.42
1:A:1685:LEU:O	1:A:1688:VAL:HG12	2.19	0.42
1:B:1348:LEU:HD21	1:B:1360:THR:HG22	2.02	0.42
1:B:1935:ALA:O	1:B:1977:TYR:HA	2.20	0.42
1:A:951:ALA:O	1:A:955:GLY:N	2.53	0.42
1:A:1225:MET:HE3	1:A:1225:MET:N	2.29	0.42
1:B:1857:ASP:OD1	1:B:1858:ALA:N	2.53	0.42
1:A:1287:ASP:O	1:A:1290:SER:OG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:THR:HG22	1:B:1129:THR:O	2.19	0.42
1:B:1408:GLU:OE1	1:B:1975:ARG:NH1	2.53	0.42
1:B:1800:PRO:O	1:B:1805:ARG:NH2	2.48	0.42
1:B:1760:LEU:CD2	1:B:1972:ARG:HE	2.33	0.42
1:A:2051:ARG:NE	1:A:2055:GLU:OE2	2.44	0.41
1:B:1660:ASP:OD1	1:B:1661:VAL:N	2.53	0.41
1:B:1873:SER:OG	1:B:1874:PRO:HD3	2.20	0.41
1:A:1319:PHE:CD2	1:A:1378:LEU:HD13	2.55	0.41
1:A:1439:SER:O	1:A:1440:ASP:C	2.63	0.41
1:B:1432:GLN:OE1	1:B:1728:ARG:NH1	2.53	0.41
1:A:1058:THR:N	1:A:1073:GLU:O	2.52	0.41
1:A:1150:GLY:O	1:A:1151:GLU:C	2.63	0.41
1:A:1763:ARG:NH1	1:A:1787:ALA:O	2.52	0.41
1:A:1785:ALA:HB3	1:A:1811:LEU:HD11	2.02	0.41
1:A:2020:LEU:CD2	1:A:2100:LEU:HD21	2.51	0.41
1:B:1771:GLY:O	1:B:1794:LEU:HD11	2.20	0.41
1:B:1803:LYS:O	1:B:1807:THR:HG23	2.20	0.41
1:A:1578:ILE:HD13	1:A:1710:LEU:HD21	2.03	0.41
1:A:1886:THR:O	1:A:1886:THR:CG2	2.68	0.41
1:A:1098:PHE:O	1:A:1099:GLN:C	2.64	0.41
1:A:1251:VAL:HG13	1:A:1251:VAL:O	2.21	0.41
1:A:1666:ARG:HG2	1:A:1666:ARG:O	2.20	0.41
1:B:1117:PRO:C	1:B:1118:LEU:HD22	2.45	0.41
1:B:1364:ASP:OD2	1:B:1390:ARG:NH1	2.53	0.41
1:B:1647:LEU:HD12	1:B:1651:GLY:C	2.45	0.41
1:A:1287:ASP:OD1	1:A:1287:ASP:C	2.63	0.41
1:A:1771:GLY:N	1:A:1795:THR:O	2.54	0.41
1:B:945:MET:HE1	1:B:977:ILE:HD11	2.01	0.41
1:A:1043:PHE:CD1	1:A:1043:PHE:C	2.98	0.41
1:B:1409:ARG:CZ	1:B:1753:VAL:HG11	2.51	0.41
1:B:1647:LEU:HD21	1:B:1676:LEU:HD21	2.03	0.41
1:A:961:ARG:O	1:A:962:ASP:OD1	2.39	0.41
1:A:1347:LEU:O	1:A:1351:ILE:HG12	2.21	0.41
1:A:1441:ARG:CZ	1:A:1516:PHE:CE2	3.04	0.41
1:B:1906:SER:HB3	1:B:1909:GLN:HG2	2.01	0.41
1:A:1591:GLY:O	1:A:1596:ARG:NH2	2.52	0.41
1:A:1848:VAL:O	1:A:1893:TRP:NE1	2.49	0.41
1:B:1190:LEU:HD21	1:B:1970:LEU:HD21	2.03	0.41
1:B:1251:VAL:C	1:B:1252:GLN:HG3	2.46	0.41
1:B:1303:ARG:NH1	1:B:1865:ASP:OD2	2.49	0.41
1:B:1590:ALA:N	1:B:1610:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:CD2	2:A:2201:MU4:C38	2.83	0.41
1:A:1920:ASP:OD2	1:A:1977:TYR:CE1	2.74	0.41
1:A:905:LEU:HD21	1:B:913:VAL:HG21	2.02	0.40
1:A:1357:MET:SD	1:A:1357:MET:C	3.04	0.40
1:A:1730:MET:SD	1:A:1739:LEU:HD23	2.61	0.40
1:B:1043:PHE:CD1	1:B:1044:ALA:N	2.89	0.40
1:B:1098:PHE:CD1	1:B:1098:PHE:C	2.97	0.40
1:B:1239:PRO:HD2	1:B:1242:THR:HG22	2.04	0.40
1:B:1282:ARG:O	1:B:1336:ARG:NH2	2.54	0.40
1:B:1980:TYR:O	1:B:1980:TYR:CG	2.74	0.40
1:B:1996:SER:N	1:B:1997:PRO:HD3	2.37	0.40
1:A:1455:MET:SD	1:A:1537:ILE:HG21	2.61	0.40
1:A:1698:LEU:HA	1:A:1701:VAL:HG22	2.03	0.40
1:A:1846:ARG:HA	1:A:1891:LEU:HD12	2.02	0.40
1:B:972:ASP:O	1:B:973:GLU:C	2.64	0.40
1:A:947:LEU:CD2	1:A:1123:LEU:HD22	2.45	0.40
1:A:1327:ILE:O	1:A:1327:ILE:HG23	2.22	0.40
1:A:1329:LYS:O	1:A:1330:PRO:C	2.65	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	1213/2124 (57%)	1099 (91%)	109 (9%)	5 (0%)	30	60
1	B	1107/2124 (52%)	1005 (91%)	99 (9%)	3 (0%)	36	65
All	All	2320/4248 (55%)	2104 (91%)	208 (9%)	8 (0%)	37	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	928	ASP
1	A	1148	ARG
1	B	1670	PHE
1	A	930	GLN
1	A	1089	ILE
1	A	1203	VAL
1	B	1053	ALA
1	B	966	GLU

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	942/1634 (58%)	931 (99%)	11 (1%)	63	71
1	B	854/1634 (52%)	852 (100%)	2 (0%)	87	86
All	All	1796/3268 (55%)	1783 (99%)	13 (1%)	73	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	930	GLN
1	A	967	GLN
1	A	968	MET
1	A	970	LEU
1	A	996	ASN
1	A	1187	SER
1	A	1188	GLU
1	A	1507	PHE
1	A	1998	TRP
1	A	2015	PHE
1	A	2060	SER
1	B	1636	THR
1	B	1760	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	912	HIS
1	A	930	GLN
1	A	933	ASN
1	A	996	ASN
1	A	1030	HIS
1	A	1032	HIS
1	A	1099	GLN
1	A	1218	ASN
1	A	1565	HIS
1	A	1573	GLN
1	B	896	HIS
1	B	1252	GLN
1	B	1300	HIS
1	B	1459	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MU4	A	2201	1	21,25,38	0.22	0	25,32,47	0.64	1 (4%)

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	MU4	A	2201	1	-	12/30/32/45	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	MU4	C31-C29-C28	2.47	112.31	108.22

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	MU4	O27-C28-C29-C30
2	A	2201	MU4	O27-C28-C29-C31
2	A	2201	MU4	O27-C28-C29-C32
2	A	2201	MU4	N36-C37-C38-C39
2	A	2201	MU4	C38-C39-N41-C42
2	A	2201	MU4	C2-C3-C4-C5
2	A	2201	MU4	O40-C39-N41-C42
2	A	2201	MU4	O14-C2-N1-C43
2	A	2201	MU4	C3-C2-N1-C43
2	A	2201	MU4	N41-C42-C43-N1
2	A	2201	MU4	O14-C2-C3-C4
2	A	2201	MU4	N1-C2-C3-C4

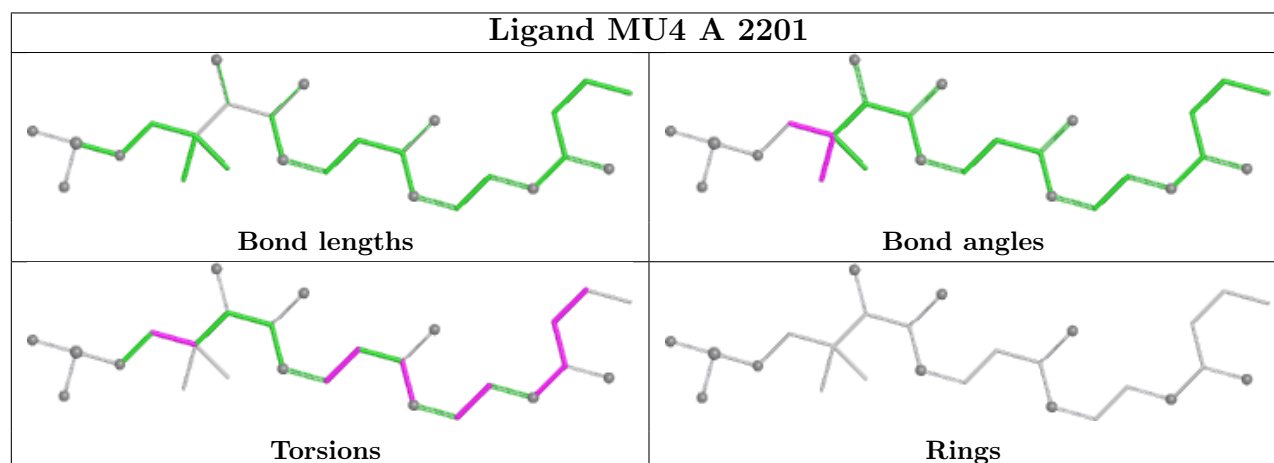
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2201	MU4	8	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.

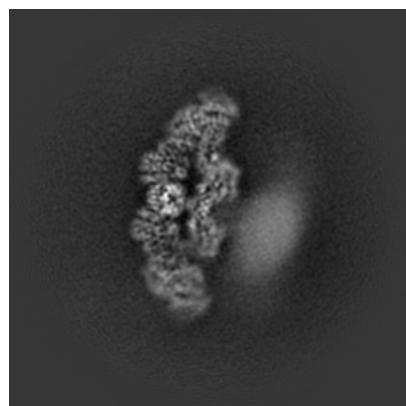
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46506. These allow visual inspection of the internal detail of the map and identification of artifacts.

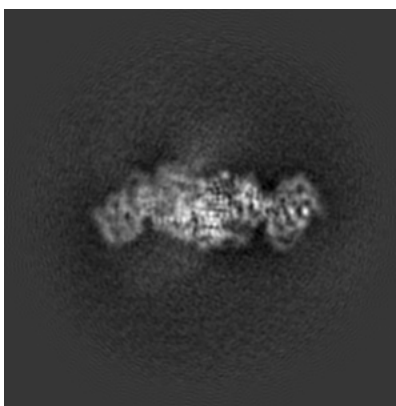
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

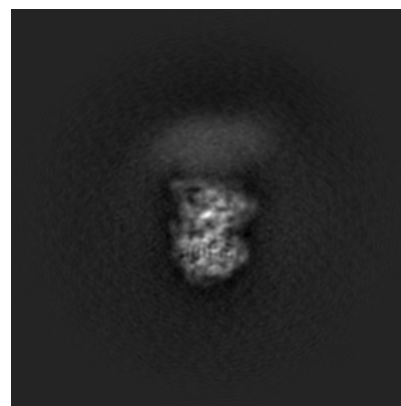
6.1.1 Primary map



X

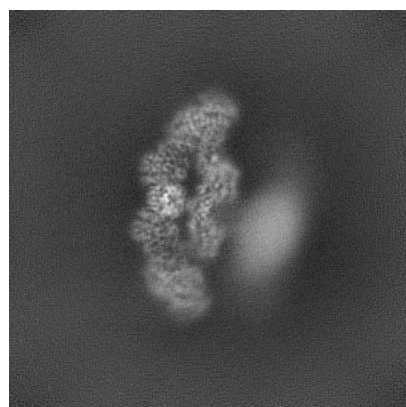


Y

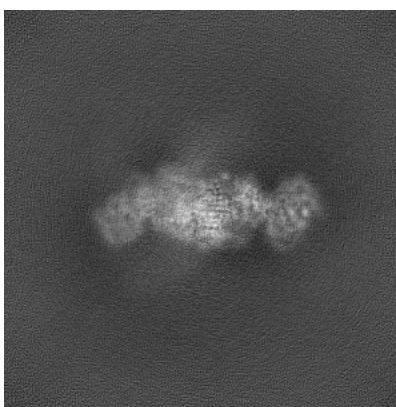


Z

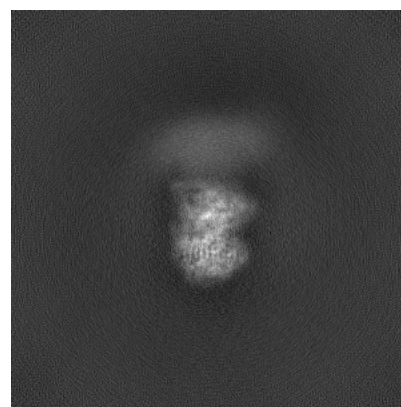
6.1.2 Raw map



X



Y

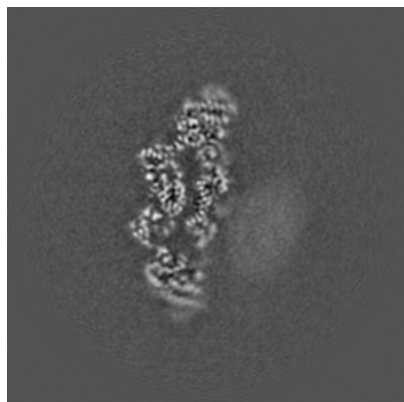


Z

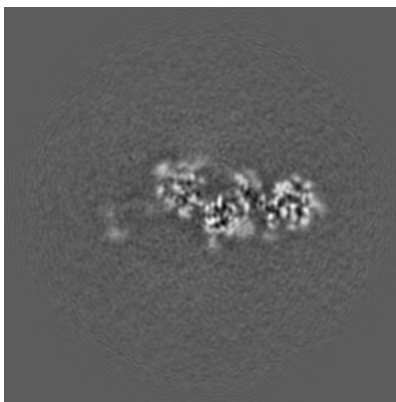
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

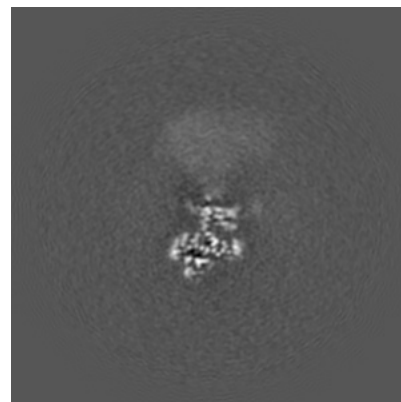
6.2.1 Primary map



X Index: 192

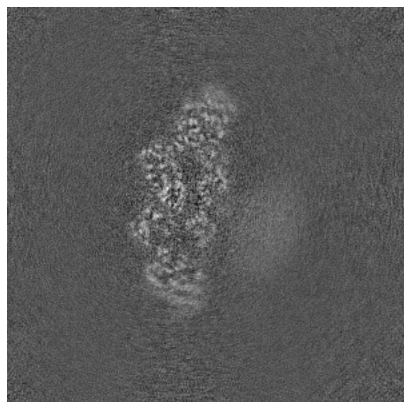


Y Index: 192

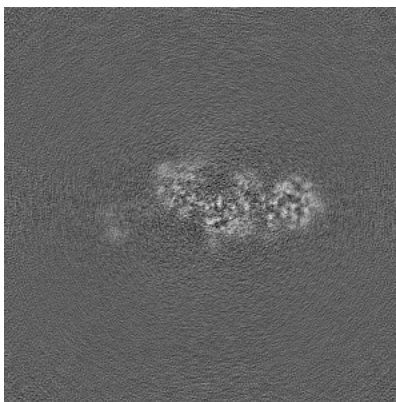


Z Index: 192

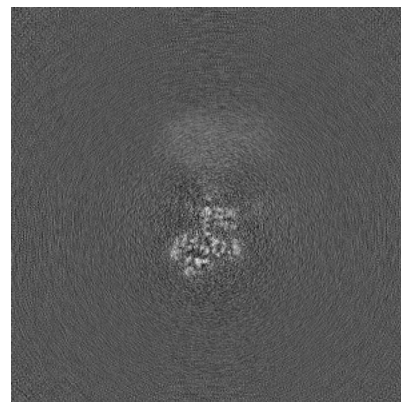
6.2.2 Raw map



X Index: 192



Y Index: 192

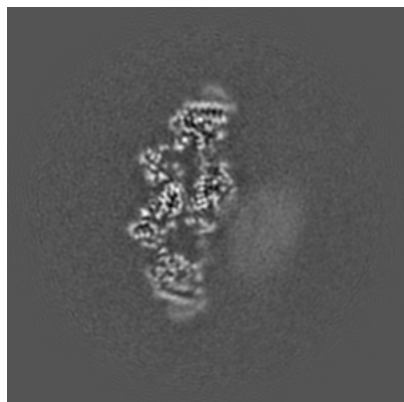


Z Index: 192

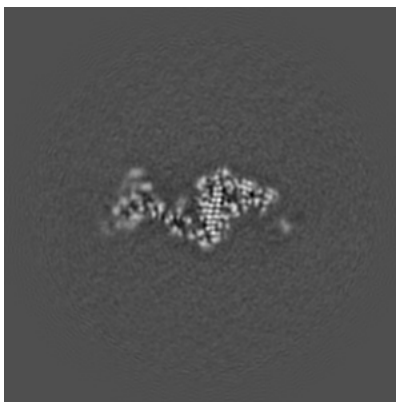
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

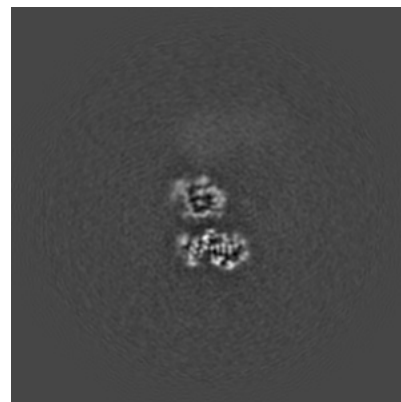
6.3.1 Primary map



X Index: 188

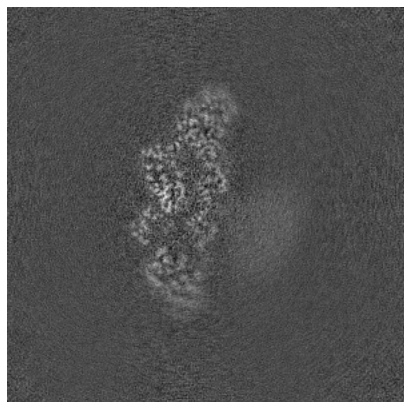


Y Index: 150

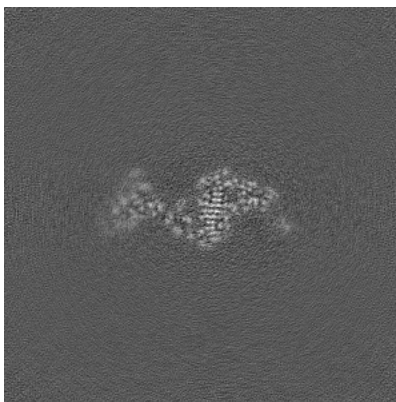


Z Index: 208

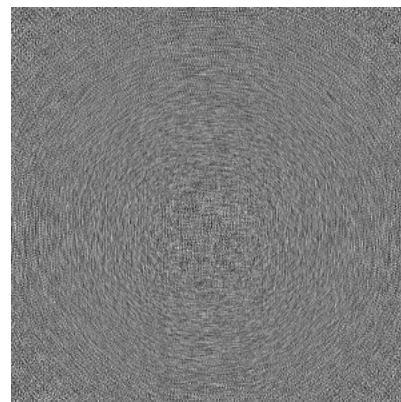
6.3.2 Raw map



X Index: 193



Y Index: 151

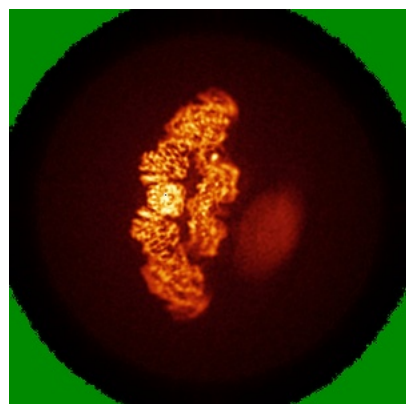


Z Index: 0

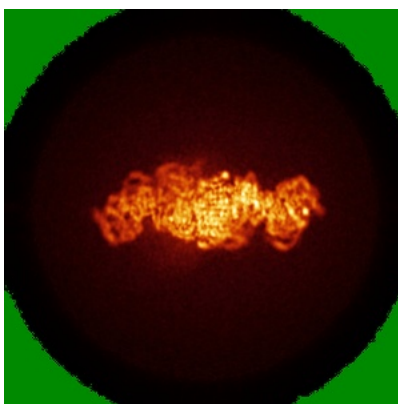
The images above show the largest variance slices of the map in three orthogonal directions.

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

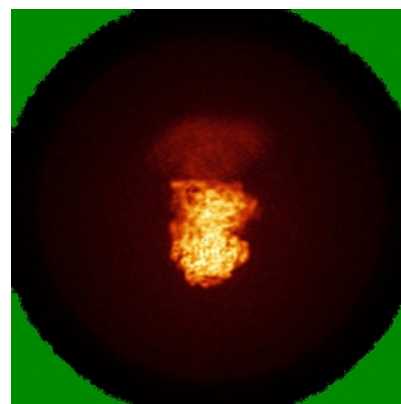
6.4.1 Primary map



X

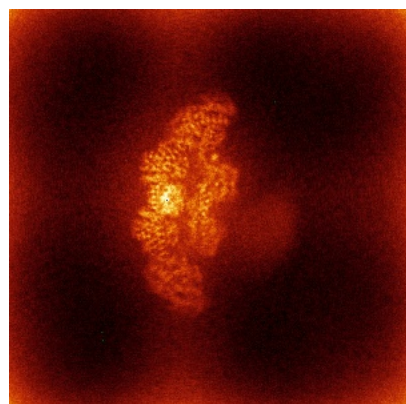


Y

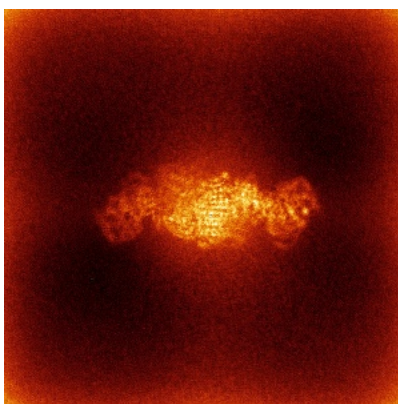


Z

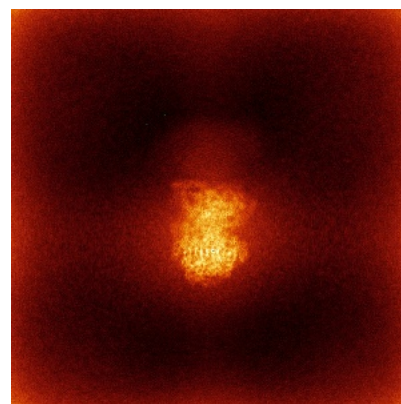
6.4.2 Raw map



X



Y

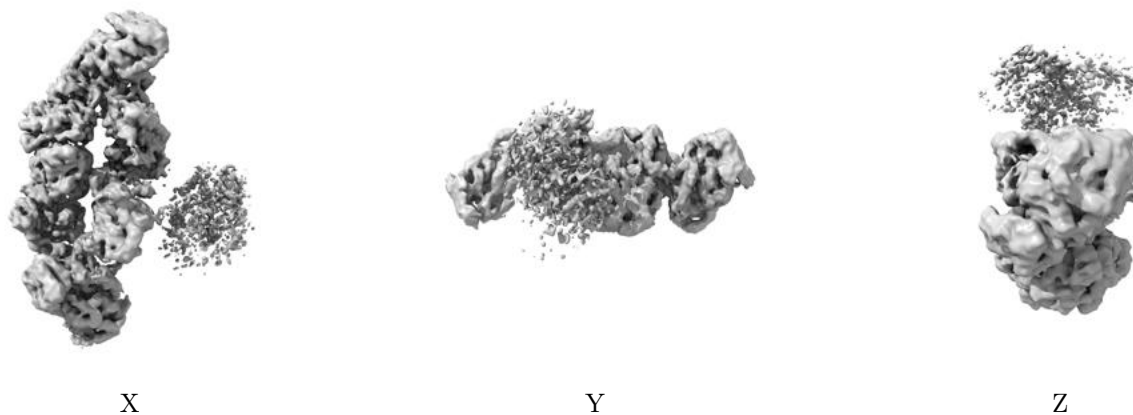


Z

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.

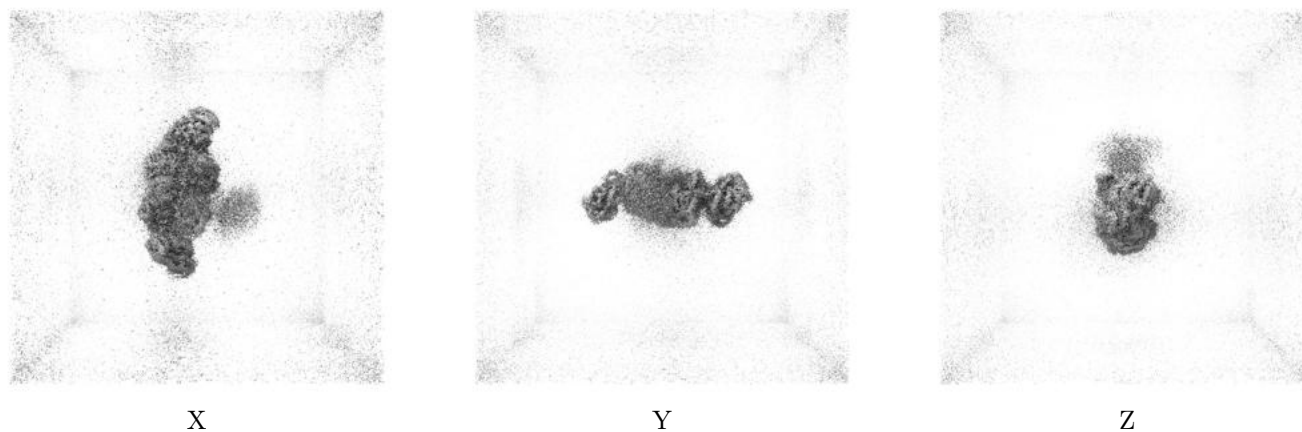
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

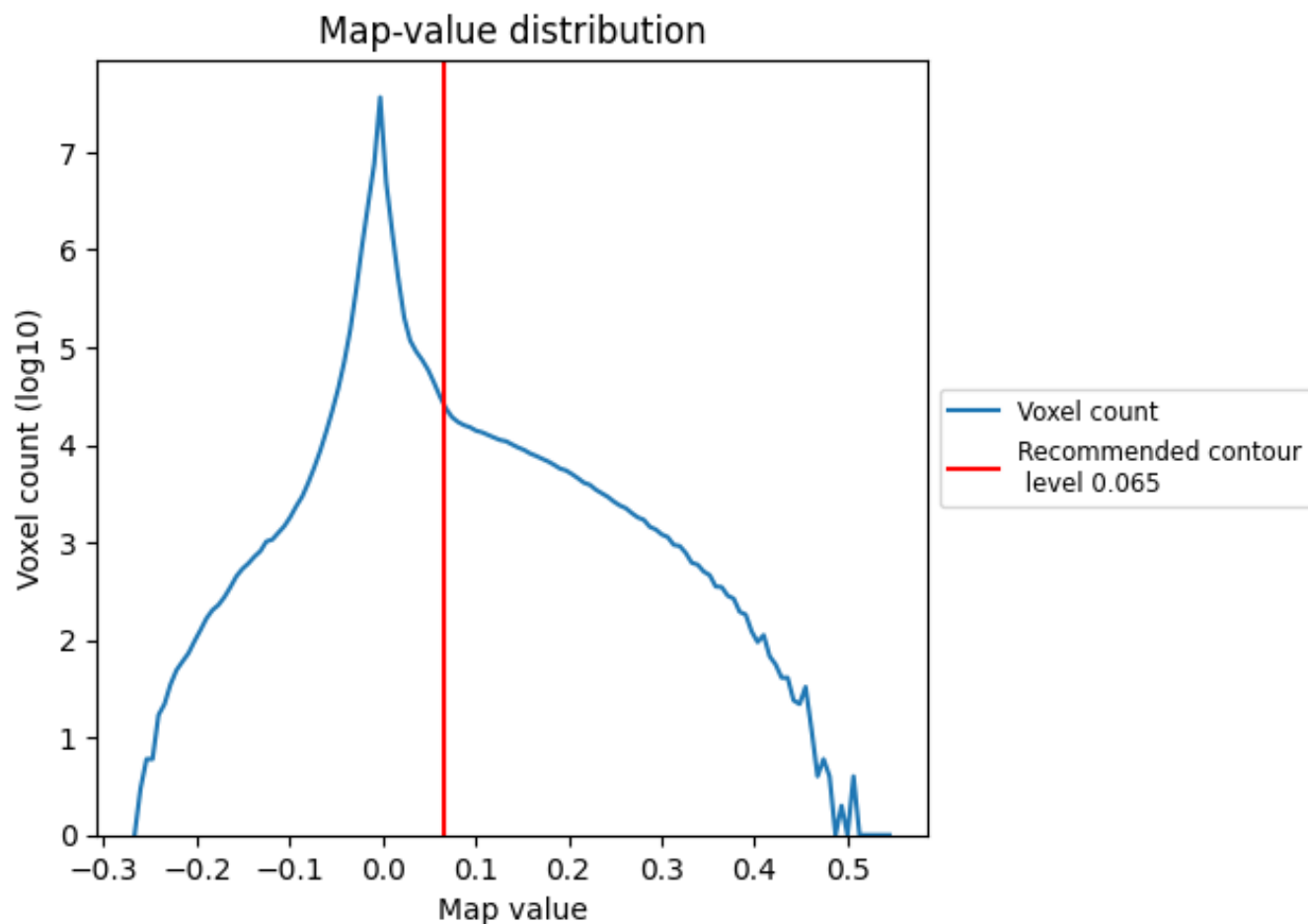
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

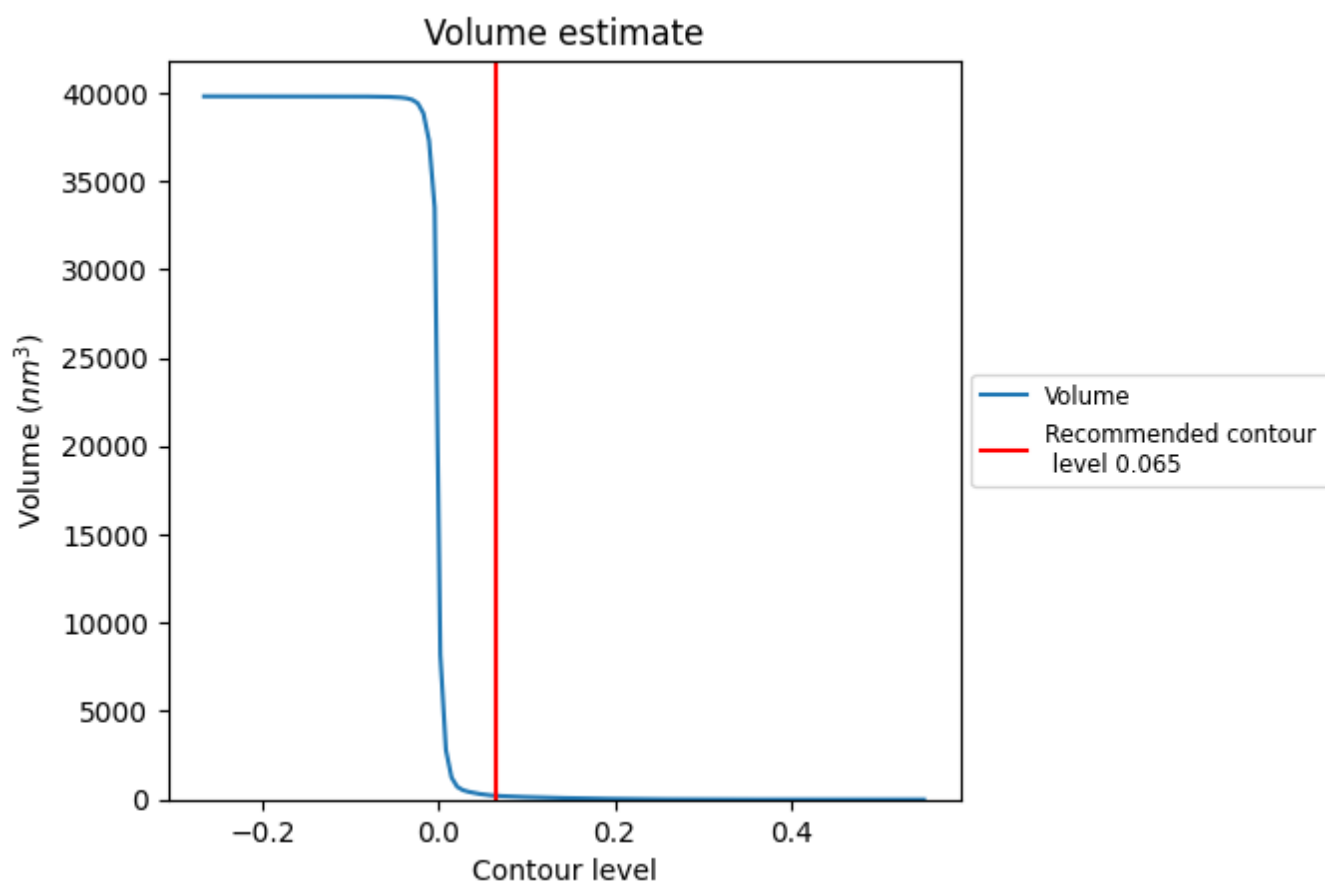
This section contains the results of statistical analysis of the map.

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.

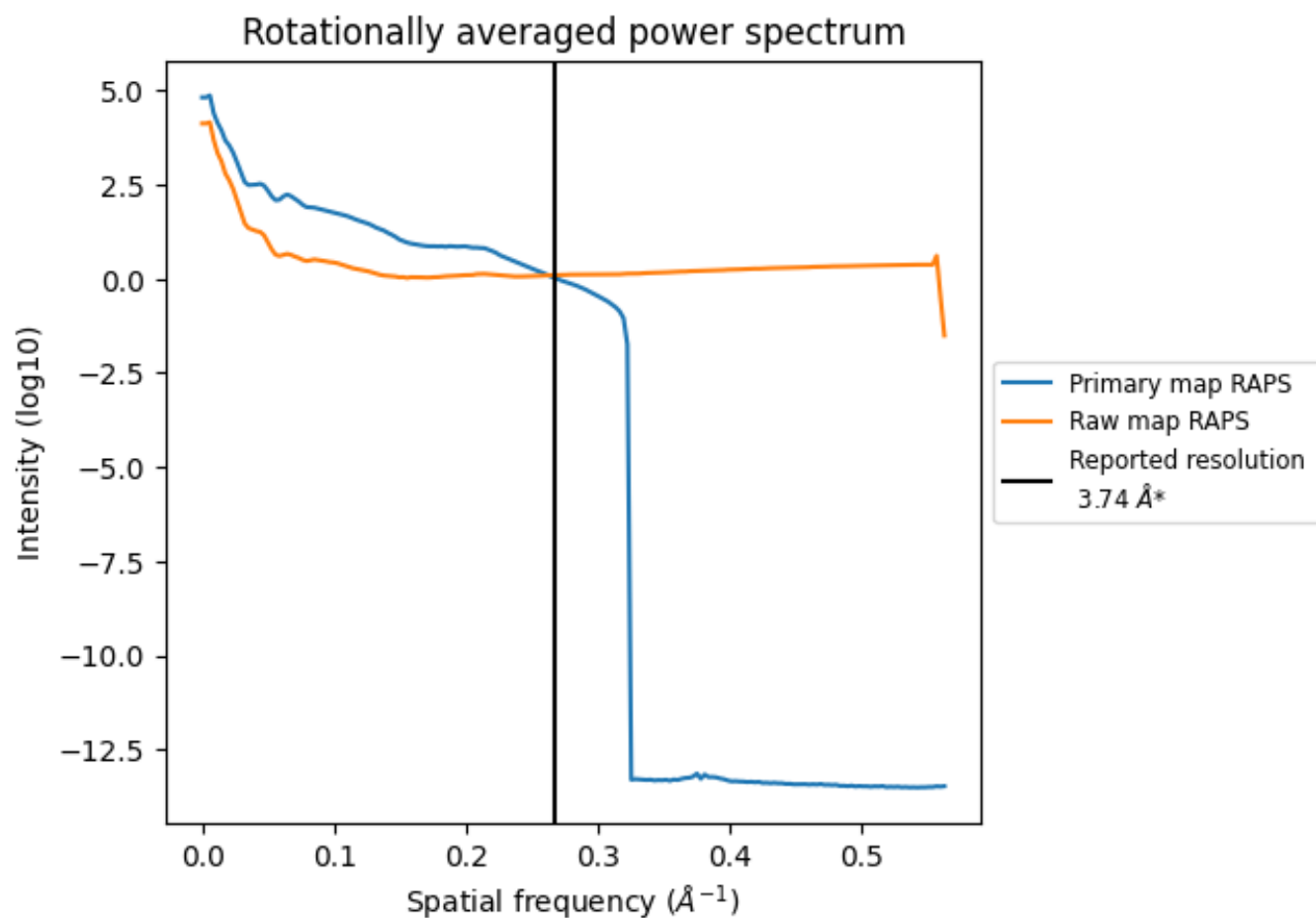
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 ⓘ

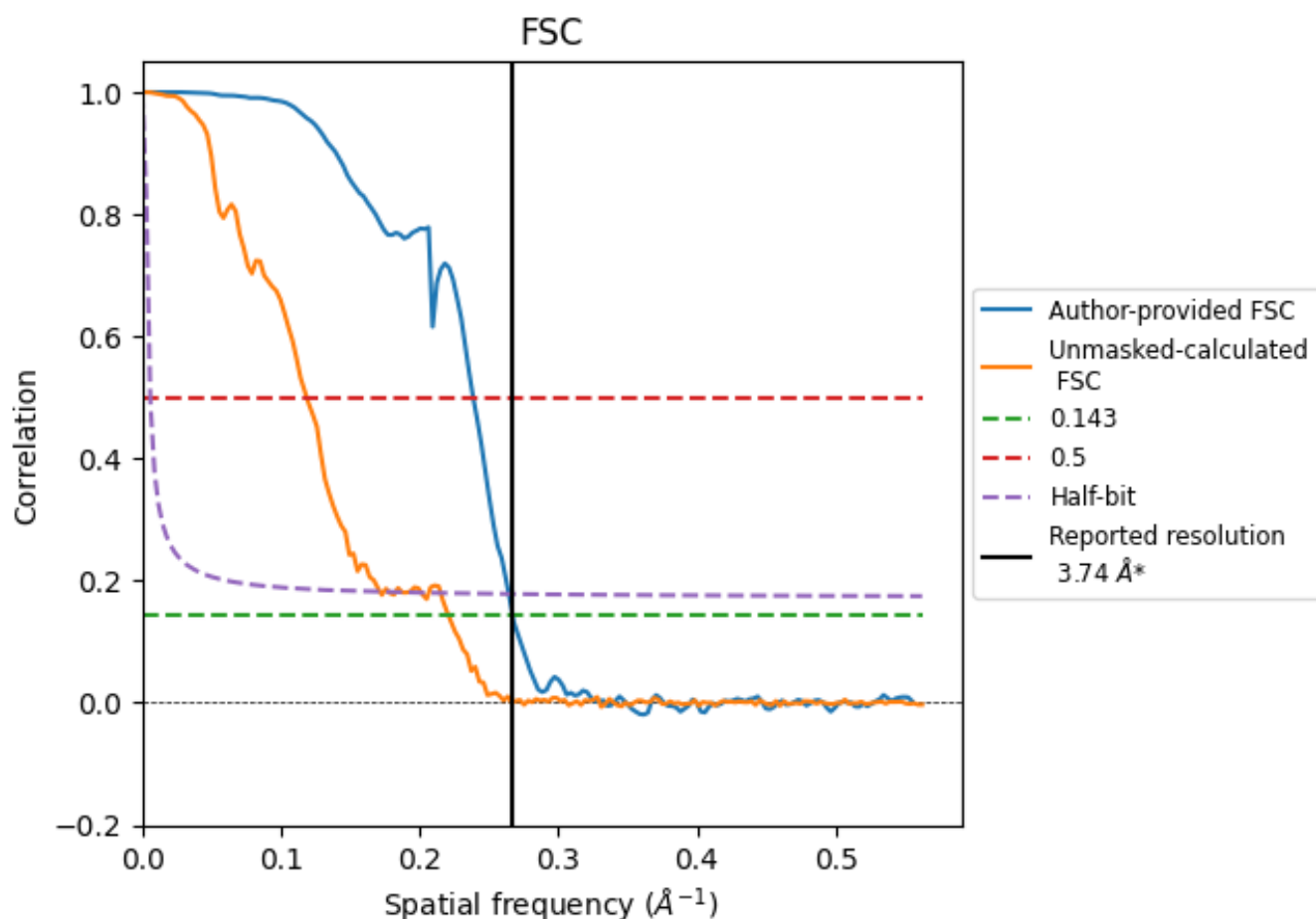


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 \AA^{-1}

8.2 Resolution estimates [i](#)

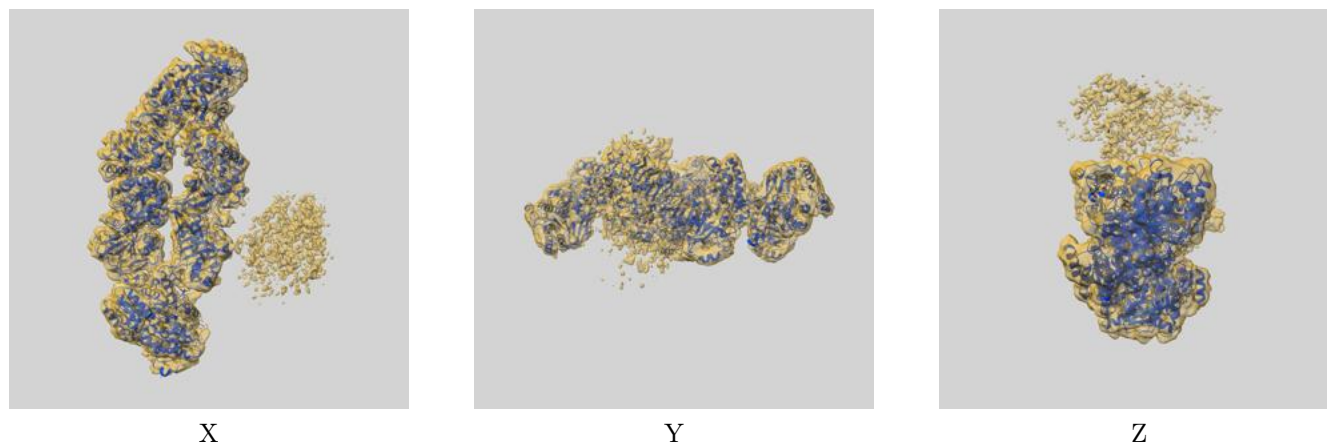
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.74	4.19	3.78
Unmasked-calculated*	4.53	8.43	5.83

*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 4.53 differs from the reported value 3.74 by more than 10 %

9 Map-model fit [i](#)

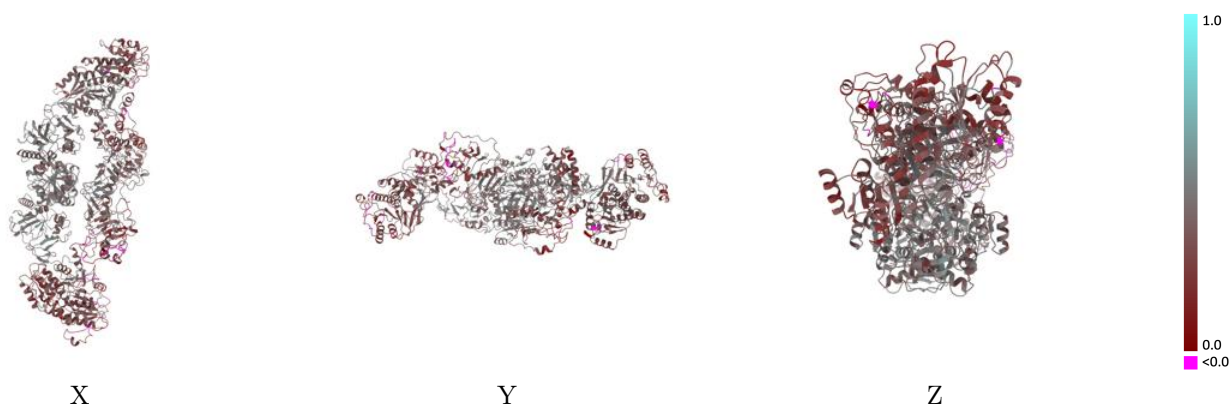
This section contains information regarding the fit between EMDB map EMD-46506 and PDB model 9D30. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



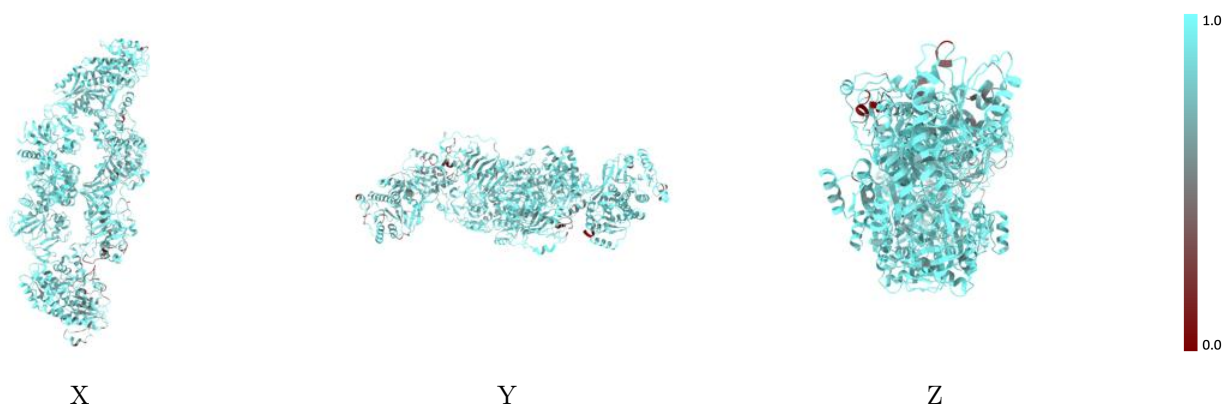
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



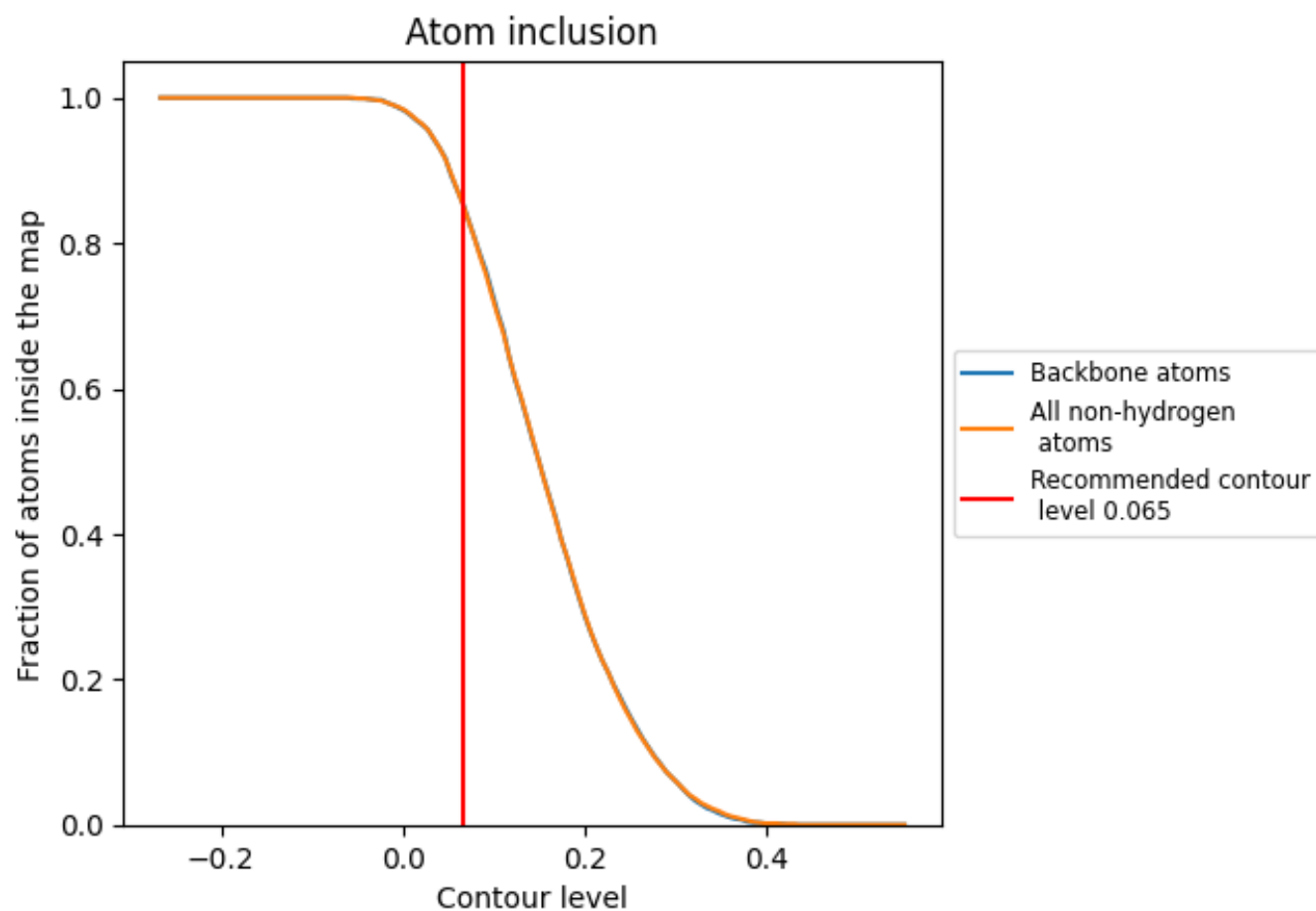
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8560	<div></div> 0.3520
A	<div></div> 0.8780	<div></div> 0.3680
B	<div></div> 0.8390	<div></div> 0.3350

