



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:05 AM UTC

PDB ID : 9CTK / pdb_00009ctk
EMDB ID : EMD-45909
Title : Modifying region of EcPKS2 - malonylCoA inhibited dataset
Authors : Schubert, H.L.; Hill, C.P.
Deposited on : 2024-07-25
Resolution : 2.92 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

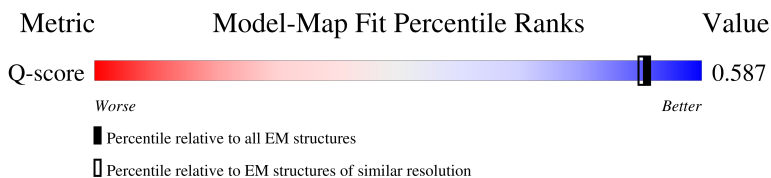
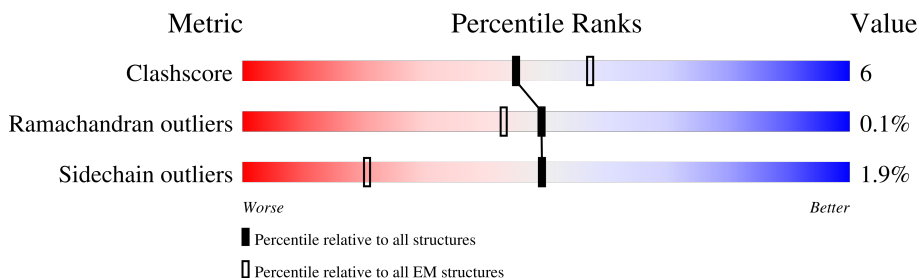
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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	2287	
1	B	2287	

Mol	Chain	Residues	Atoms		AltConf
3	A	110	Total 110	O 110	0
3	B	112	Total 112	O 112	0

E2125	R1939	E1687	M1471	L1290	E1185	ALA	ALA	GLY	GLY	VAL	VAL	GLY	VAL	LEU	ARG	SER	ALA	GLY	SER	ILE
K2126	R1943	V1698	L1474	V1291	N1186	ILE	GLN	GLU	THR	GLN	GLN	GLU	VAL	VAL	GLN	GLY	ASN	THR	ILE	TYR
R2131	L1970	L1701	R1475	M1292	D1187	ILE	PHE	ALA	GLY	PHE	ALA	ALA	ALA	HIS	GLU	GLY	ALA	GLY	HIS	LYS
D2134	V1971	A1706	F1478	V1295	K1188	VAL	VAL	VAL	D972	R972	VAL	VAL	VAL	CYS	LEU	PRO	PRO	ILE	ILE	LYS
G2135	M1974	A1709	I1486	S1296	N1189	ILE	ILE	GLY	G874	G874	ALA	ALA	ALA	GLY	GLY	SER	LEU	SER	ALA	ASP
L2136	M1977	T1709	I1487	D1297	N1190	ASP	ASP	ASP	E975	E975	GLY	GLY	GLY	VAL	VAL	LEU	ALA	VAL	ASP	ASP
T2140	M1977	S1717	C1494	V1299	V1191	THR	THR	THR	S985	S985	LEU	LEU	GLN	GLY	CYS	TYR	ILE	ILE	ASN	ASN
I2146	E1980	L1718	L1497	Q1302	P1193	PRO	PRO	PRO	T993	T993	MET	MET	VAL	VAL	VAL	ALA	ALA	THR	ASP	THR
V2149	R1988	V1733	L1497	V1303	N1194	LEU	LEU	LEU	D994	D994	SER	SER	VAL	VAL	VAL	VAL	VAL	GLY	ASP	VAL
THR	R1988	P1734	E1498	M1304	E1196	SER	SER	SER	L1003	L1003	SER	SER	ILE	ILE	ILE	ILE	ILE	THR	GLY	LYS
VAL	T1994	A1760	E1499	K1331	E1197	LYS	LYS	LYS	L1011	L1011	MET	MET	LYS	LYS	LYS	GLY	GLY	THR	ARG	THR
ALA	L1995	S1763	Q1501	M1354	I1198	VAL	VAL	VAL	L1012	L1012	SER	SER	GLY	GLY	GLY	ALA	ALA	THR	ASP	ASP
LEU	T1996	V1764	A1502	D1360	K1199	SER	SER	GLY	E1020	E1020	ALA	ALA	GLN	GLN	GLN	THR	THR	PRO	ILE	HIS
MET	S1987	F1781	L1516	P1361	H1207	THR	THR	THR	G1034	G1034	ASP	ASP	GLY	GLY	GLY	ARG	ARG	PRO	PRO	PRO
GLY	R2008	T1782	L1524	A1362	H1208	CYS	CYS	CYS	G1051	G1051	THR	THR	GLU	GLU	GLU	LEU	LEU	ASN	ASN	ASN
THR	K2009	L1783	L1548	N1363	A1209	ILE	ILE	ILE	S1039	S1039	VAL	VAL	VAL	TRP	TRP	LEU	LEU	ASP	ASP	ASP
ASN	E2021	D1802	I1548	E1367	THR	ALA	ALA	ALA	D1044	D1044	LYS	LYS	GLY	GLY	GLY	GLY	GLY	LYS	LYS	LYS
GLY	H2039	C1806	G1554	L1368	GLN	TRP	TRP	TRP	D1050	D1050	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	PRO	PRO
T2161	K2042	S1807	P1555	T1369	ALA	ALA	ALA	ALA	G1051	G1051	ARG	ARG	GLN	GLU	GLU	GLU	GLU	ASN	ASN	ASN
Q2169	M2052	E1809	N1556	E1370	SER	SER	SER	SER	S1055	S1055	PRO	PRO	GLN	GLU	GLU	LEU	LEU	PRO	PRO	PRO
V2174	A2053	D1810	K1569	L1374	N1217	LEU	LEU	LEU	S1055	S1055	VAL	VAL	GLN	GLU	GLU	LEU	LEU	ILE	ILE	ILE
D2179	M2054	F1813	I1560	L1375	F1218	GLU	GLU	GLU	T1089	T1089	PRO	PRO	ALA	ALA	ALA	ALA	ALA	GLY	GLY	GLY
M2182	V2055	E1814	F1567	L1377	A1219	PHE	PHE	PHE	V1082	V1082	ASN	ASN	THR	THR	THR	THR	THR	PHE	PHE	PHE
D2185	M2064	R1818	V1571	L1381	S1220	LEU	LEU	LEU	P1090	P1090	TYR	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
V2193	N2065	N1831	R1572	L1404	L1225	GLY	GLY	GLY	A1091	A1091	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V2201	F2069	K1839	K1573	L1413	V1229	SER	SER	SER	Q1092	Q1092	PHE	PHE	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ALA	L2070	A1840	D1574	L1419	N1230	GLY	GLY	GLY	E1099	E1099	SER	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ALA	E2074	S1841	N1578	I1419	N1231	SER	SER	SER	L1103	L1103	ALA	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
GLY	M2079	R1842	R1598	K1420	N1233	ALA	ALA	ALA	K1106	K1106	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	L2083	L1845	R1602	A1421	G1234	GLY	GLY	GLY	E1120	E1120	LYS	LYS	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
SER	S2087	F1851	A1609	L1427	H1235	CYS	CYS	CYS	D888	D888	ILE	ILE	SER	SER	SER	SER	SER	SER	SER	SER
VAL	R2088	K1857	S1638	K1430	H1236	LEU	LEU	LEU	D1136	D1136	THR	THR	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
ASP	V2100	D1879	L1658	A1438	H1240	VAL	VAL	VAL	D1142	D1142	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
VAL	M2101	Q1885	I1662	M1439	F1243	PRO	PRO	PRO	F1143	F1143	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
ARG	S2104	L1892	I1668	F1442	L1256	ASN	ASN	ASN	R1156	R1156	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
ALA	L2105	V1896	E1675	Y1443	G1256	PRO	PRO	PRO	E1174	E1174	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
VAL	I2106	V1896	E1675	H1468	D1257	GLY	GLY	GLY	F1175	F1175	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
GLY	V2107	K1933	G1685	V1469	Y1258	ASN	ASN	ASN	S1176	S1176	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	Q2114		V1686	S1470	W1259	TYR	TYR	TYR	L1177	L1177	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
VAL					D1260	PRO	PRO	PRO	N951	N951	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
					L1261															
					L1262															
					H1267															
					L1282															

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	258974	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.781	Depositor
Minimum map value	-1.815	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.286	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	3/10483 (0.0%)	0.59	10/14194 (0.1%)
1	B	0.29	3/10483 (0.0%)	0.50	7/14194 (0.0%)
All	All	0.34	6/20966 (0.0%)	0.55	17/28388 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2192	TYR	C-O	-8.55	1.13	1.23
1	A	2190	ILE	C-O	-6.18	1.17	1.24
1	B	1813	PHE	C-O	-5.09	1.17	1.24
1	B	1831	ASN	C-O	-5.05	1.17	1.24
1	B	1841	SER	CA-CB	-5.05	1.46	1.53
1	A	1813	PHE	C-O	-5.02	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1781	PHE	CA-C-O	-7.42	112.34	120.36
1	B	1781	PHE	CA-C-O	-7.38	112.39	120.36
1	A	2192	TYR	CA-C-O	-6.73	113.45	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2110	GLY	CA-C-O	-6.41	117.10	122.29
1	A	1578	ASN	CA-C-O	-5.88	114.01	120.30
1	B	1809	GLU	N-CA-CB	-5.56	101.76	110.44
1	A	2065	ASN	CA-C-O	-5.55	115.10	121.82
1	B	1302	GLN	N-CA-C	-5.51	107.10	113.88
1	B	1839	LYS	CA-C-O	-5.51	115.02	120.70
1	A	1809	GLU	N-CA-CB	-5.51	101.84	110.44
1	A	1839	LYS	CA-C-O	-5.47	115.07	120.70
1	A	1302	GLN	N-CA-C	-5.42	107.21	113.88
1	B	2065	ASN	CA-C-O	-5.38	115.31	121.82
1	B	1194	ASN	CA-C-O	-5.21	114.34	120.81
1	A	1810	ASP	CA-C-O	-5.19	115.90	121.45
1	B	1810	ASP	CA-C-O	-5.16	115.92	121.45
1	A	2036	VAL	CA-C-O	-5.14	115.07	120.57

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1263	ARG	Sidechain
1	A	1503	ARG	Sidechain
1	A	1544	ARG	Sidechain
1	B	1503	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	10247	10221	10221	128	0
1	B	10247	10221	10221	129	0
2	A	48	25	25	0	0
2	B	48	25	25	3	0
3	A	110	0	0	4	0
3	B	112	0	0	4	0
All	All	20812	20492	20492	257	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 6.

All (257) 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:B:1478:PHE:CG	1:B:1574:ASP:OD2	1.90	1.25
1:B:1478:PHE:CD2	1:B:1574:ASP:OD2	1.96	1.18
1:A:1417:PHE:HE1	1:A:1427:LEU:HD11	1.34	0.92
1:B:1262:LEU:HD23	1:B:1422:ILE:HG21	1.50	0.91
1:B:1478:PHE:CB	1:B:1574:ASP:OD2	2.23	0.86
1:A:1427:LEU:HD23	1:A:1427:LEU:O	1.75	0.86
1:A:1417:PHE:CE1	1:A:1427:LEU:HD11	2.15	0.81
1:A:1709:THR:O	1:A:1939:ARG:NH2	2.17	0.78
1:A:1598[B]:ARG:NH2	3:A:5104:HOH:O	2.23	0.72
1:B:1764:VAL:HG11	1:B:1933:LYS:HG2	1.72	0.72
1:A:1764:VAL:HG11	1:A:1933:LYS:HG2	1.72	0.71
1:B:1598[B]:ARG:NH2	3:B:5104:HOH:O	2.23	0.69
1:A:1609:ALA:O	3:A:5101:HOH:O	2.11	0.69
1:A:1267:HIS:O	1:A:1267:HIS:ND1	2.26	0.69
1:B:1609:ALA:O	3:B:5101:HOH:O	2.10	0.69
1:A:1487:ILE:HD12	1:A:1516:LEU:HD11	1.75	0.68
1:A:1971:VAL:HG21	1:A:2083:LEU:HD11	1.75	0.68
1:A:993:THR:OG1	1:A:1120:GLU:OE2	2.11	0.68
1:B:1267:HIS:O	1:B:1267:HIS:ND1	2.26	0.68
1:B:1839:LYS:HE3	1:B:1842[A]:ARG:NH2	2.09	0.67
1:A:2021:GLU:OE1	1:A:2042:LYS:NZ	2.28	0.67
1:B:2021:GLU:OE1	1:B:2042:LYS:NZ	2.28	0.66
1:B:993:THR:OG1	1:B:1120:GLU:OE2	2.11	0.66
1:B:1709:THR:O	1:B:1939:ARG:NH2	2.28	0.66
1:A:1839:LYS:HE3	1:A:1842[A]:ARG:NH2	2.09	0.66
1:A:1439:MET:SD	1:A:1439:MET:N	2.69	0.65
1:B:1192:LEU:HD12	1:B:1259:TRP:HE1	1.61	0.65
1:B:1051:GLY:O	1:B:1092:GLN:NE2	2.30	0.64
1:A:1051:GLY:O	1:A:1092:GLN:NE2	2.31	0.64
1:A:2146:ILE:HD12	1:A:2174:VAL:HG21	1.81	0.63
1:A:1354:MET:HE1	1:A:1368:LEU:HD21	1.80	0.63
1:B:1971:VAL:HG21	1:B:2083:LEU:HD11	1.79	0.63
1:B:1258:TYR:CE1	1:B:1262:LEU:HD22	2.33	0.63
1:A:1438:ALA:N	1:A:1442:PHE:O	2.32	0.63
1:B:1354:MET:HE1	1:B:1368:LEU:HD21	1.81	0.62
1:B:2146:ILE:HD12	1:B:2174:VAL:HG21	1.81	0.62
1:B:1478:PHE:HB3	1:B:1574:ASP:OD2	1.99	0.61
1:B:1438:ALA:N	1:B:1442:PHE:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2100:VAL:O	1:B:2101:MET:HE2	2.02	0.60
1:A:1143:PHE:O	3:A:5102:HOH:O	2.16	0.59
1:A:2105:LEU:HD12	1:A:2108:SER:HB3	1.83	0.59
1:A:2021:GLU:OE2	1:A:2039:HIS:ND1	2.36	0.59
1:B:2021:GLU:OE2	1:B:2039:HIS:ND1	2.36	0.59
1:A:1845:LEU:HD11	1:A:1851:PHE:HB2	1.83	0.59
1:A:2100:VAL:O	1:A:2101:MET:HE2	2.02	0.59
1:B:1845:LEU:HD11	1:B:1851:PHE:HB2	1.84	0.59
1:A:1460:ILE:HG23	1:A:1575:LEU:HD11	1.85	0.58
1:A:1544:ARG:NH2	1:A:1574:ASP:O	2.37	0.58
1:B:1294:THR:O	1:B:1298:ASN:ND2	2.37	0.56
1:A:1662:ILE:HG21	1:A:1668:ILE:HD12	1.88	0.56
1:B:1143:PHE:O	3:B:5102:HOH:O	2.17	0.56
1:A:1783:LEU:HD23	1:A:1806:CYS:HB2	1.88	0.56
1:B:1439:MET:SD	1:B:1439:MET:N	2.80	0.55
1:B:1487:ILE:HD12	1:B:1516:LEU:HD11	1.88	0.55
1:B:1258:TYR:CZ	1:B:1262:LEU:HD22	2.42	0.55
1:A:2088:ARG:NH1	1:A:2134:ASP:OD2	2.40	0.54
1:B:1783:LEU:HD23	1:B:1806:CYS:HB2	1.88	0.54
1:B:2087:SER:OG	1:B:2131:ARG:NH1	2.40	0.54
1:A:1012:LEU:HD11	1:A:2008:ARG:HD2	1.90	0.54
1:B:1354:MET:HE1	1:B:1368:LEU:HD11	1.90	0.54
1:B:2079:MET:SD	2:B:5001:NAP:N6A	2.81	0.54
1:B:1225:LEU:HD13	1:B:1243:PHE:CD1	2.43	0.54
1:B:1662:ILE:HG21	1:B:1668:ILE:HD12	1.88	0.54
1:B:1494:CYS:HB2	1:B:2070:LEU:HD11	1.90	0.54
1:A:2087:SER:OG	1:A:2131:ARG:NH1	2.41	0.54
1:B:1034:GLY:HA3	1:B:1059:THR:HG21	1.90	0.54
1:A:1687:GLU:OE2	1:A:1933:LYS:NZ	2.32	0.54
1:A:1034:GLY:HA3	1:A:1059:THR:HG21	1.90	0.53
1:A:1225:LEU:HD13	1:A:1243:PHE:CD1	2.43	0.53
1:A:1494:CYS:HB2	1:A:2070:LEU:HD11	1.91	0.53
1:B:1012:LEU:HD11	1:B:2008:ARG:HD2	1.90	0.53
1:A:1354:MET:HE1	1:A:1368:LEU:HD11	1.91	0.53
1:B:2054:MET:SD	1:B:2056:LEU:HD13	2.49	0.53
1:B:1194:ASN:ND2	1:B:1427:LEU:HD12	2.23	0.53
1:B:1687:GLU:OE2	1:B:1933:LYS:NZ	2.32	0.53
1:A:1197:GLU:HG3	1:A:1427:LEU:HD22	1.90	0.53
1:A:1717:SER:OG	1:A:1885:GLN:NE2	2.40	0.53
1:A:1003:LEU:HB3	1:A:1011:LEU:HD21	1.91	0.53
1:B:2088:ARG:NH1	1:B:2134:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ASP:OD1	1:A:957:THR:OG1	2.28	0.52
1:B:1422:ILE:HG22	1:B:1422:ILE:O	2.09	0.52
1:B:1997:SER:OG	2:B:5001:NAP:O3X	2.24	0.52
1:B:1003:LEU:HB3	1:B:1011:LEU:HD21	1.92	0.52
1:A:2105:LEU:HD13	1:A:2190:ILE:CG2	2.40	0.52
1:B:888:ASP:OD1	1:B:957:THR:OG1	2.26	0.52
1:B:1567:PHE:O	1:B:1571:VAL:HG23	2.10	0.52
1:B:2125:GLU:HG3	1:B:2140:THR:HG21	1.92	0.52
1:A:1567:PHE:O	1:A:1571:VAL:HG23	2.10	0.52
1:B:1839:LYS:HE3	1:B:1842[A]:ARG:HH22	1.74	0.52
1:A:2054:MET:SD	1:A:2056:LEU:HD13	2.50	0.51
1:B:1292:MET:HE1	1:B:1374:LEU:HD21	1.92	0.51
1:B:2146:ILE:CD1	1:B:2174:VAL:HG21	2.41	0.51
1:A:1988:ARG:NH2	1:A:2179:ASP:OD2	2.44	0.51
1:A:2105:LEU:HD13	1:A:2190:ILE:HG21	1.93	0.51
1:B:1020:GLU:OE2	1:B:2008:ARG:NH1	2.45	0.50
1:A:917:LEU:HD13	1:A:1082:VAL:HG11	1.94	0.50
1:A:1020:GLU:OE2	1:A:2008:ARG:NH1	2.44	0.50
1:A:2146:ILE:CD1	1:A:2174:VAL:HG21	2.40	0.50
1:A:2125:GLU:HG3	1:A:2140:THR:HG21	1.92	0.50
1:B:1497:LEU:HD11	1:B:1501:GLN:NE2	2.27	0.50
1:B:1717:SER:OG	1:B:1885:GLN:NE2	2.40	0.50
1:A:1974:MET:HE3	1:A:2022:VAL:HG11	1.93	0.50
1:B:1988:ARG:NH2	1:B:2179:ASP:OD2	2.44	0.50
1:B:1290:LEU:O	1:B:1294:THR:OG1	2.25	0.49
1:A:1191:VAL:O	1:A:1191:VAL:HG22	2.13	0.49
1:A:1292:MET:HE1	1:A:1374:LEU:HD21	1.93	0.49
1:A:1839:LYS:HE3	1:A:1842[A]:ARG:HH22	1.74	0.49
1:A:1247:ASP:OD1	1:A:1251:SER:OG	2.26	0.49
1:A:1469:VAL:HG12	1:A:1470:SER:N	2.27	0.49
1:B:1050:ASP:OD1	1:B:1050:ASP:N	2.45	0.49
1:A:1044:ASP:OD1	1:A:1106:LYS:NZ	2.41	0.49
1:A:1698:VAL:HB	1:A:1718:LEU:HD22	1.94	0.49
1:B:1469:VAL:HG12	1:B:1470:SER:N	2.28	0.49
1:A:1377:LEU:HD13	1:A:1381:LEU:HD13	1.94	0.49
1:B:1191:VAL:HG22	1:B:1191:VAL:O	2.13	0.48
1:A:1295:VAL:O	1:A:1299:VAL:HG13	2.13	0.48
1:A:1436:ASP:OD1	1:A:1436:ASP:N	2.46	0.48
1:B:1486:ILE:HD11	1:B:1567:PHE:CE2	2.48	0.48
1:A:1257:ASP:O	1:A:1261:ARG:NH1	2.47	0.48
1:B:917:LEU:HD13	1:B:1082:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1291:VAL:O	1:B:1295:VAL:HG23	2.14	0.48
1:A:1497:LEU:HD11	1:A:1501:GLN:NE2	2.28	0.48
1:B:2136:LEU:O	3:B:5103:HOH:O	2.20	0.48
1:B:1257:ASP:O	1:B:1261:ARG:NH1	2.47	0.48
1:A:1486:ILE:HD11	1:A:1567:PHE:CE2	2.49	0.48
1:B:1377:LEU:HD13	1:B:1381:LEU:HD13	1.94	0.48
1:B:1698:VAL:HB	1:B:1718:LEU:HD22	1.94	0.47
1:A:884:ASP:O	1:A:885:ASN:C	2.57	0.47
1:A:1427:LEU:O	1:A:1427:LEU:CD2	2.54	0.47
1:B:1662:ILE:CG2	1:B:1668:ILE:HD12	2.45	0.47
1:A:973:ASP:C	1:A:973:ASP:OD1	2.57	0.47
1:A:1012:LEU:HD12	1:A:1039:SER:O	2.15	0.47
1:A:1050:ASP:OD1	1:A:1050:ASP:N	2.45	0.47
1:B:1174:GLU:OE2	1:B:1177:ARG:NH1	2.48	0.47
1:B:1370:GLU:OE1	1:B:1370:GLU:N	2.48	0.47
1:A:1197:GLU:CG	1:A:1427:LEU:HD22	2.45	0.47
1:B:973:ASP:OD1	1:B:973:ASP:C	2.57	0.47
1:A:1291:VAL:O	1:A:1295:VAL:HG23	2.15	0.47
1:A:1518:LEU:HD12	1:A:1531:LEU:HD12	1.97	0.47
1:A:1662:ILE:CG2	1:A:1668:ILE:HD12	2.45	0.47
1:B:1136:ASP:OD1	1:B:1136:ASP:N	2.39	0.47
1:B:1375:LEU:HD23	1:B:1404:LEU:CD1	2.45	0.47
1:B:1814:GLU:OE2	1:B:1818[B]:ARG:NH2	2.48	0.47
1:A:2136:LEU:O	3:A:5103:HOH:O	2.20	0.47
1:A:1174:GLU:OE2	1:A:1177:ARG:NH1	2.48	0.47
1:A:2107:VAL:HG11	1:A:2125:GLU:OE2	2.14	0.47
1:A:1152:ARG:NH2	1:A:1582:ASN:O	2.45	0.46
1:A:1370:GLU:N	1:A:1370:GLU:OE1	2.48	0.46
1:A:1814:GLU:OE2	1:A:1818[B]:ARG:NH2	2.48	0.46
1:B:884:ASP:O	1:B:885:ASN:C	2.57	0.46
1:A:1255:GLU:OE2	1:A:1261:ARG:NH2	2.49	0.46
1:A:1295:VAL:HG12	1:A:1304:MET:HE3	1.98	0.46
1:A:1375:LEU:HD23	1:A:1404:LEU:CD1	2.45	0.46
1:A:1687:GLU:HB3	1:A:1701:LEU:HD23	1.98	0.46
1:A:1377:LEU:HD13	1:A:1381:LEU:CD1	2.46	0.45
1:B:1475:ARG:NH1	1:B:1573:LYS:O	2.43	0.45
1:B:1857:LYS:H	1:B:1857:LYS:HD2	1.81	0.45
1:A:1760:ALA:O	1:A:1763:SER:OG	2.33	0.45
1:A:1857:LYS:H	1:A:1857:LYS:HD2	1.80	0.45
1:B:1175:PHE:CD2	1:B:1225:LEU:HD12	2.50	0.45
1:B:1255:GLU:OE2	1:B:1261:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:TYR:CE1	1:A:1262:LEU:HD22	2.52	0.45
1:A:1361:PRO:O	1:A:1362:ALA:HB3	2.16	0.45
1:A:2064:MET:HE3	1:A:2069:PHE:HD1	1.81	0.45
1:B:1012:LEU:HD12	1:B:1039:SER:O	2.16	0.45
1:B:894:ASP:OD1	1:B:894:ASP:N	2.48	0.45
1:B:1455:HIS:N	1:B:1455:HIS:CD2	2.85	0.45
1:A:2100:VAL:CG2	1:A:2182:MET:HE3	2.47	0.45
1:B:1361:PRO:O	1:B:1362:ALA:HB3	2.15	0.45
1:B:2100:VAL:HG21	1:B:2182:MET:HE3	1.98	0.45
1:A:1417:PHE:CE1	1:A:1427:LEU:CD1	2.96	0.45
1:B:916:THR:HB	1:B:971:VAL:HG21	1.99	0.45
1:B:1377:LEU:HD13	1:B:1381:LEU:CD1	2.47	0.45
1:B:1571:VAL:O	1:B:1574:ASP:OD1	2.33	0.45
1:B:1044:ASP:OD1	1:B:1106:LYS:NZ	2.41	0.45
1:B:1524:LEU:HD22	1:B:2127:ILE:HG13	1.99	0.45
1:A:1548:ILE:HD11	1:A:1560:ILE:HG12	1.99	0.44
1:B:2100:VAL:CG2	1:B:2182:MET:HE3	2.47	0.44
1:A:894:ASP:OD1	1:A:894:ASP:N	2.48	0.44
1:A:916:THR:HB	1:A:971:VAL:HG21	1.99	0.44
1:B:1295:VAL:HG12	1:B:1304:MET:HE3	1.99	0.44
1:B:2106:ILE:HD11	1:B:2114:GLN:O	2.18	0.44
1:A:1455:HIS:N	1:A:1455:HIS:CD2	2.83	0.44
1:A:1524:LEU:HD22	1:A:2127:ILE:HG13	1.99	0.44
1:A:1282:LEU:HD13	1:A:1471:MET:HB2	2.00	0.44
1:A:1475:ARG:NH1	1:A:1573:LYS:O	2.44	0.44
1:B:1687:GLU:HB3	1:B:1701:LEU:HD23	1.98	0.44
1:B:1055:SER:O	1:B:1059:THR:HG23	2.18	0.44
1:B:1421:ALA:HA	1:B:1427:LEU:HD11	1.99	0.44
1:A:1638:SER:OG	1:A:1675:GLU:OE2	2.28	0.44
1:A:2100:VAL:HG21	1:A:2182:MET:HE3	1.98	0.44
1:B:951:ASN:OD1	1:B:951:ASN:N	2.51	0.44
1:B:1282:LEU:HD13	1:B:1471:MET:HB2	1.99	0.44
1:A:1980:GLU:OE2	1:A:2009:LYS:NZ	2.51	0.43
1:B:1879:ASP:OD1	1:B:1879:ASP:N	2.51	0.43
1:A:1970:LEU:HB2	1:A:1995:LEU:HD23	2.01	0.43
1:B:1142:ASP:OD2	1:B:1156:ARG:NH1	2.51	0.43
1:B:1487:ILE:HG21	1:B:1500:VAL:HG22	2.00	0.43
1:B:2064:MET:HE3	1:B:2069:PHE:HD1	1.83	0.43
1:A:1180:MET:HE1	1:A:1201:ALA:CB	2.48	0.43
1:B:1548:ILE:HD11	1:B:1560:ILE:HG12	2.00	0.43
1:B:1638:SER:OG	1:B:1675:GLU:OE2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1760:ALA:O	1:B:1763:SER:OG	2.33	0.43
1:A:975:GLU:HA	1:A:975:GLU:OE2	2.19	0.43
1:A:1003:LEU:HD21	1:A:1044:ASP:HB2	2.01	0.43
1:A:1857:LYS:HD2	1:A:1857:LYS:N	2.33	0.43
1:A:1090:PRO:HG3	1:A:1103:LEU:HD21	2.01	0.43
1:A:1142:ASP:OD2	1:A:1156:ARG:NH1	2.51	0.43
1:A:1291:VAL:HG12	1:A:1292:MET:HE2	2.01	0.42
1:B:1685:GLY:C	1:B:1706:ALA:HB3	2.44	0.42
1:A:1055:SER:O	1:A:1059:THR:HG23	2.18	0.42
1:A:1259:TRP:CE2	1:A:1422:ILE:HD13	2.53	0.42
1:A:1503:ARG:HG3	1:A:1503:ARG:HH11	1.85	0.42
1:B:1857:LYS:HD2	1:B:1857:LYS:N	2.33	0.42
1:A:951:ASN:OD1	1:A:951:ASN:N	2.51	0.42
1:B:1090:PRO:HG3	1:B:1103:LEU:HD21	2.01	0.42
1:B:1733:VAL:N	1:B:1734:PRO:HD2	2.35	0.42
1:B:1413:LEU:HD12	1:B:1413:LEU:H	1.84	0.42
1:B:1980:GLU:OE2	1:B:2009:LYS:NZ	2.52	0.42
1:A:1886:GLY:O	1:A:1890:THR:HG23	2.19	0.42
1:B:1003:LEU:HD21	1:B:1044:ASP:HB2	2.01	0.42
1:A:1658:LEU:HG	1:A:1662:ILE:HD13	2.01	0.42
1:A:1685:GLY:C	1:A:1706:ALA:HB3	2.45	0.42
1:B:1977:MET:HE3	2:B:5001:NAP:O4D	2.20	0.42
1:A:1413:LEU:H	1:A:1413:LEU:HD12	1.84	0.42
1:A:1879:ASP:N	1:A:1879:ASP:OD1	2.51	0.42
1:B:1970:LEU:HB2	1:B:1995:LEU:HD23	2.01	0.42
1:A:935:LEU:HD11	1:A:985:SER:OG	2.20	0.41
1:B:2107:VAL:HG11	1:B:2125:GLU:OE2	2.20	0.41
1:B:2074:GLU:O	1:B:2079:MET:HG3	2.21	0.41
1:A:994:ASP:OD1	1:A:994:ASP:C	2.63	0.41
1:B:1478:PHE:CD2	1:B:1574:ASP:CG	2.89	0.41
1:B:1658:LEU:HG	1:B:1662:ILE:HD13	2.01	0.41
1:B:1892:LEU:O	1:B:1896:VAL:HG23	2.21	0.41
1:B:2104:SER:OG	1:B:2106:ILE:HG22	2.20	0.41
1:B:935:LEU:HD11	1:B:985:SER:OG	2.20	0.41
1:B:994:ASP:OD1	1:B:994:ASP:C	2.63	0.41
1:B:1099:GLU:OE1	1:B:1099:GLU:C	2.63	0.41
1:B:1175:PHE:CD1	1:B:1175:PHE:C	2.99	0.41
1:A:1617:MET:O	1:A:1620:LEU:HD12	2.21	0.41
1:A:1733:VAL:N	1:A:1734:PRO:HD2	2.34	0.41
1:A:2074:GLU:O	1:A:2079:MET:HG3	2.21	0.41
1:A:1487:ILE:HG21	1:A:1500:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:GLU:OE2	1:B:975:GLU:HA	2.21	0.41
1:A:1099:GLU:C	1:A:1099:GLU:OE2	2.64	0.40
1:A:1892:LEU:O	1:A:1896:VAL:HG23	2.21	0.40
1:A:2023:LEU:HB3	1:A:2025:LEU:HD23	2.03	0.40
1:B:917:LEU:HD21	1:B:942:VAL:HG11	2.03	0.40
1:B:1295:VAL:O	1:B:1299:VAL:HG13	2.21	0.40
1:A:917:LEU:HD21	1:A:942:VAL:HG11	2.03	0.40
1:A:1018:TYR:CZ	1:A:1033:GLN:HA	2.56	0.40
1:B:1229:VAL:HG22	1:B:1240:HIS:CG	2.56	0.40
1:B:2169:GLN:HG2	1:B:2193:VAL:HG23	2.02	0.40
1:A:1275:ASP:OD1	1:A:1318:ARG:NH2	2.48	0.40
1:B:1503:ARG:HH11	1:B:1503:ARG:HG3	1.86	0.40
1:B:1419:ILE:HD13	1:B:1419:ILE:HA	1.97	0.40
1:B:1974:MET:HB2	1:B:1997:SER:HB2	2.03	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	1298/2287 (57%)	1252 (96%)	44 (3%)	2 (0%)	43	71
1	B	1298/2287 (57%)	1252 (96%)	45 (4%)	1 (0%)	48	76
All	All	2596/4574 (57%)	2504 (96%)	89 (3%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1468	ALA
1	B	1468	ALA
1	A	1193	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1112/1930 (58%)	1089 (98%)	23 (2%)	47	76
1	B	1112/1930 (58%)	1091 (98%)	21 (2%)	50	78
All	All	2224/3860 (58%)	2180 (98%)	44 (2%)	49	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1183	TRP
1	A	1296	SER
1	A	1331	LYS
1	A	1332	ASP
1	A	1418	PRO
1	A	1424	SER
1	A	1474	LEU
1	A	1475	ARG
1	A	1498	GLU
1	A	1531	LEU
1	A	1540	SER
1	A	1545	CYS
1	A	1574	ASP
1	A	1602	ARG
1	A	1662	ILE
1	A	1802	ASP
1	A	1808	SER
1	A	1842[A]	ARG
1	A	1842[B]	ARG
1	A	1933	LYS
1	A	1994	ILE
1	A	1997	SER
1	A	2052	MET
1	B	910	LEU
1	B	1296	SER
1	B	1331	LYS
1	B	1422	ILE

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Mol	Chain	Res	Type
1	B	1443	TYR
1	B	1474	LEU
1	B	1475	ARG
1	B	1498	GLU
1	B	1578	ASN
1	B	1602	ARG
1	B	1662	ILE
1	B	1802	ASP
1	B	1808	SER
1	B	1842[A]	ARG
1	B	1842[B]	ARG
1	B	1933	LYS
1	B	1994	ILE
1	B	1996	THR
1	B	2052	MET
1	B	2105	LEU
1	B	2185	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	995	GLN
1	A	1125	HIS
1	A	1501	GLN
1	A	1877	GLN
1	B	995	GLN
1	B	1125	HIS
1	B	1194	ASN
1	B	1501	GLN
1	B	1767	GLN
1	B	1877	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](#)

2 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
2	NAP	A	5001	-	50,52,52	0.71	1 (2%)	71,80,80	0.84	2 (2%)
2	NAP	B	5001	-	50,52,52	1.68	4 (8%)	71,80,80	1.01	4 (5%)

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	NAP	A	5001	-	-	7/35/67/67	0/5/5/5
2	NAP	B	5001	-	-	8/35/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	NAP	P2B-O2B	8.24	1.74	1.59
2	B	5001	NAP	PA-O3	4.97	1.64	1.59
2	B	5001	NAP	PN-O3	4.47	1.64	1.59
2	A	5001	NAP	C2N-N1N	3.22	1.38	1.35
2	B	5001	NAP	O4D-C1D	-2.46	1.37	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	NAP	P2B-O2B-C2B	-3.86	113.11	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	NAP	P2B-O2B-C2B	-2.86	115.78	123.43
2	A	5001	NAP	C6N-N1N-C2N	-2.83	119.47	121.88
2	B	5001	NAP	O2N-PN-O1N	2.22	122.75	112.44
2	B	5001	NAP	O4B-C1B-N9A	2.20	112.31	108.09
2	B	5001	NAP	O3X-P2B-O2X	2.16	115.91	107.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	NAP	C5B-O5B-PA-O3
2	A	5001	NAP	C5D-O5D-PN-O3
2	A	5001	NAP	C5D-O5D-PN-O1N
2	B	5001	NAP	C5B-O5B-PA-O1A
2	B	5001	NAP	C5D-O5D-PN-O3
2	B	5001	NAP	C5D-O5D-PN-O1N
2	B	5001	NAP	O4B-C4B-C5B-O5B
2	B	5001	NAP	C3B-C4B-C5B-O5B
2	B	5001	NAP	PA-O3-PN-O5D
2	B	5001	NAP	C4B-C5B-O5B-PA
2	A	5001	NAP	C4B-C5B-O5B-PA
2	A	5001	NAP	C5B-O5B-PA-O1A
2	A	5001	NAP	C5D-O5D-PN-O2N
2	B	5001	NAP	C5D-O5D-PN-O2N
2	A	5001	NAP	O4B-C4B-C5B-O5B

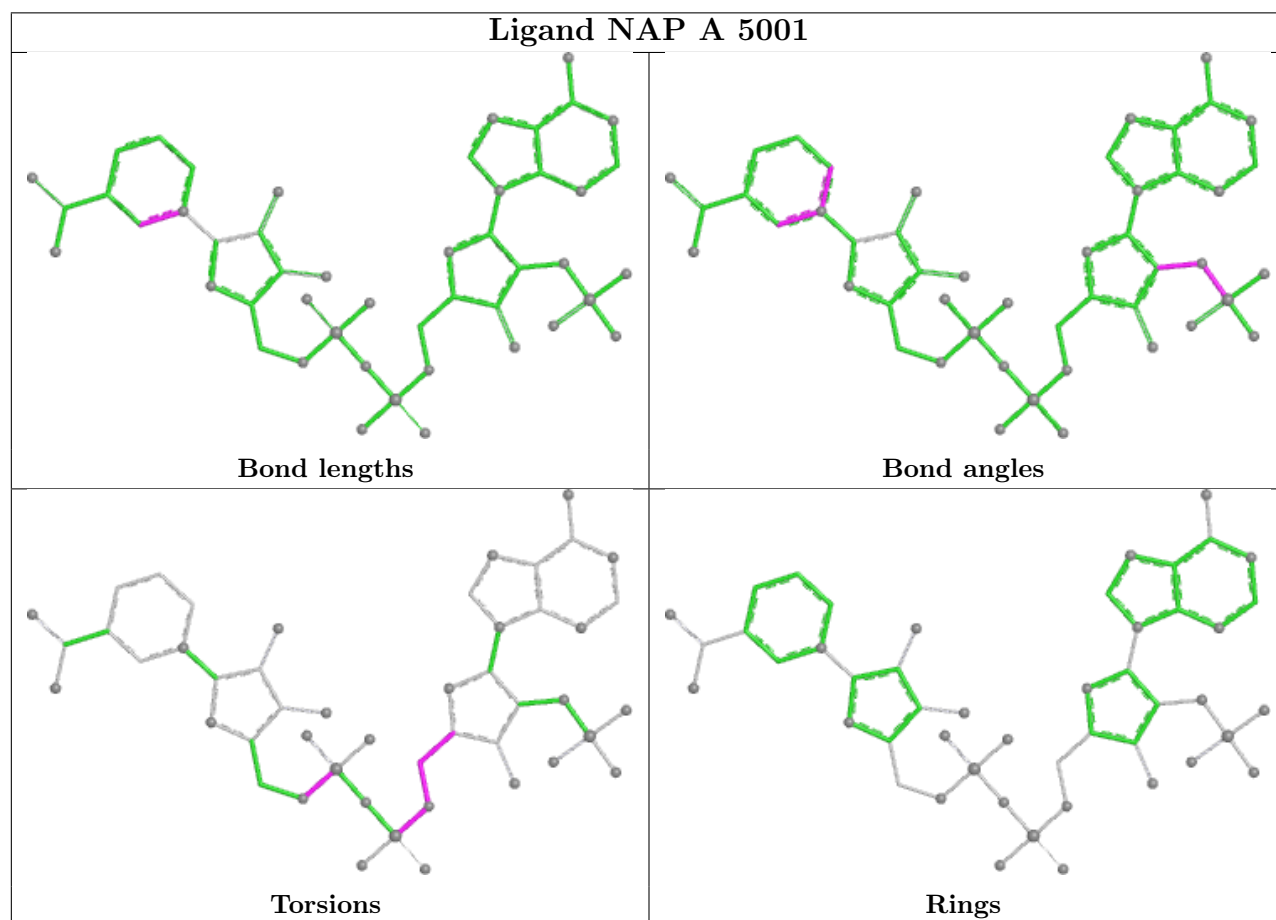
There are no ring outliers.

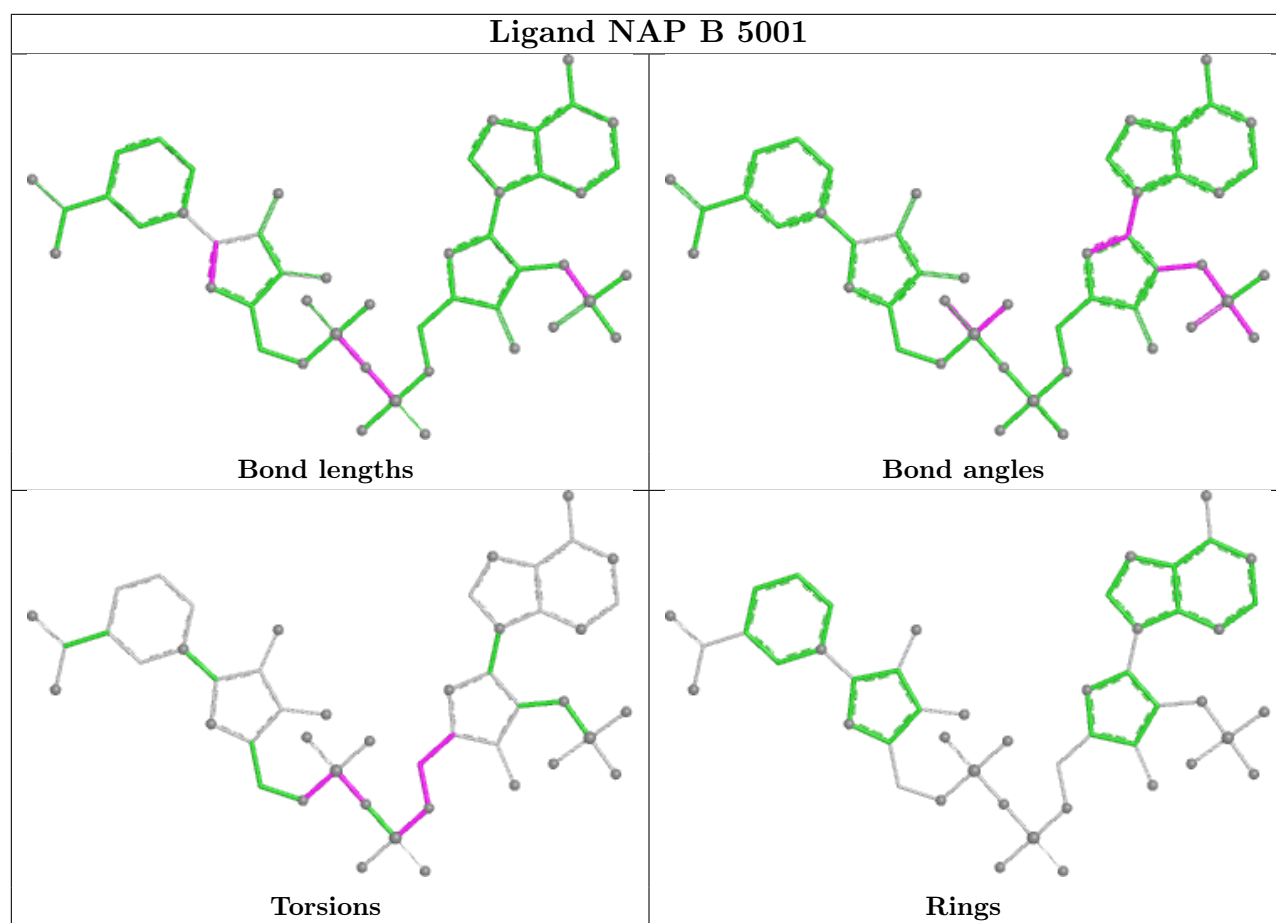
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5001	NAP	3	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.

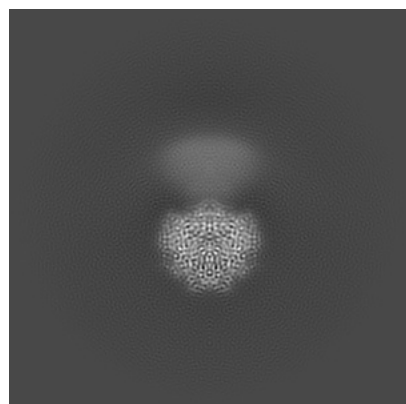
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45909. These allow visual inspection of the internal detail of the map and identification of artifacts.

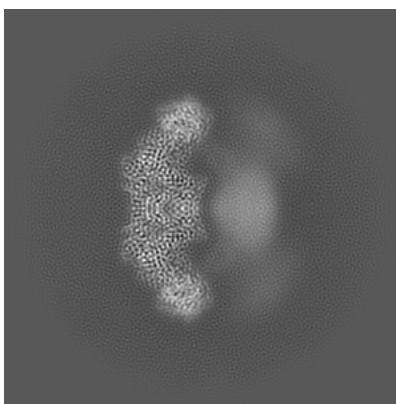
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

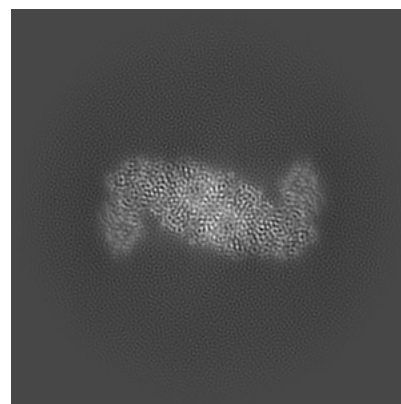
6.1.1 Primary map



X

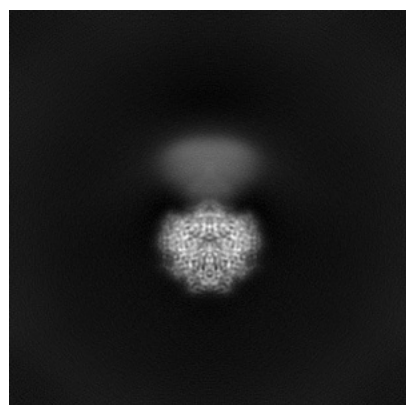


Y

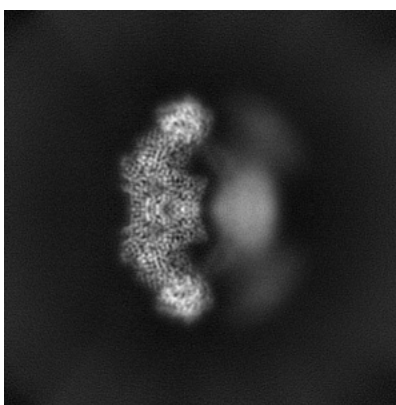


Z

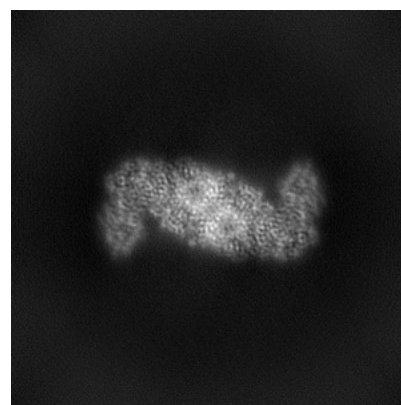
6.1.2 Raw map



X



Y

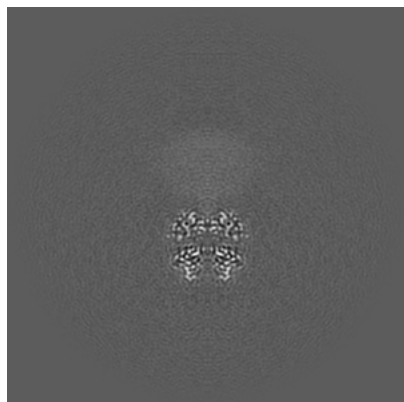


Z

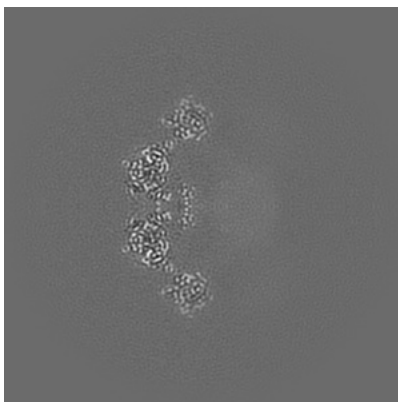
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

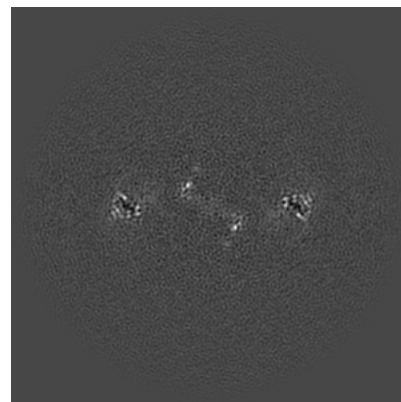
6.2.1 Primary map



X Index: 160

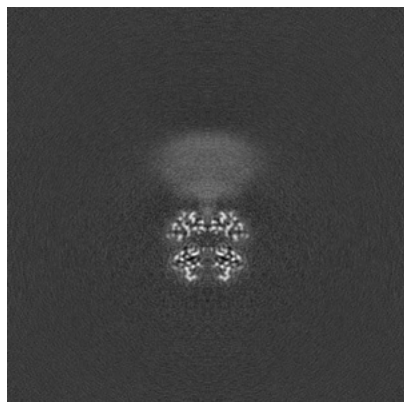


Y Index: 160

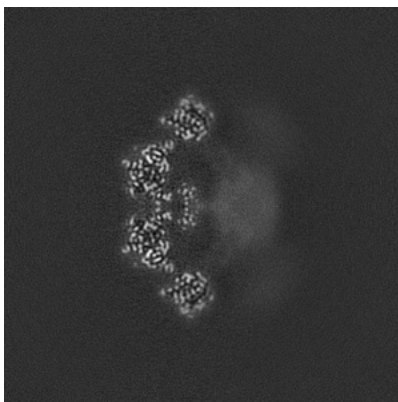


Z Index: 160

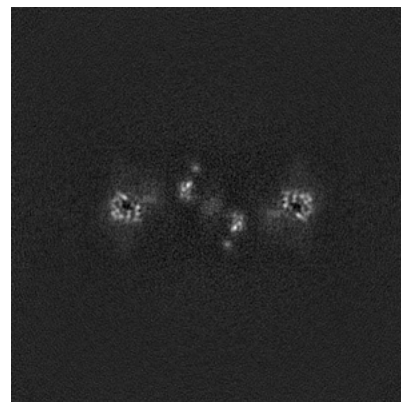
6.2.2 Raw map



X Index: 160



Y Index: 160

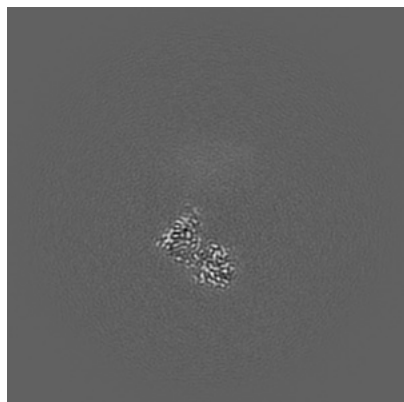


Z Index: 160

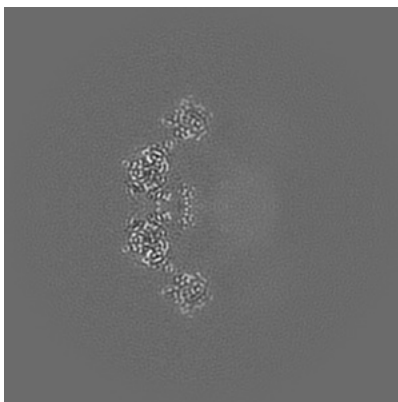
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

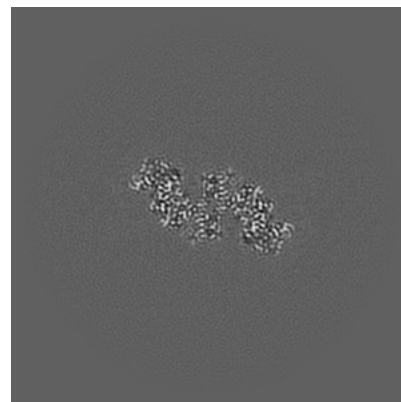
6.3.1 Primary map



X Index: 185

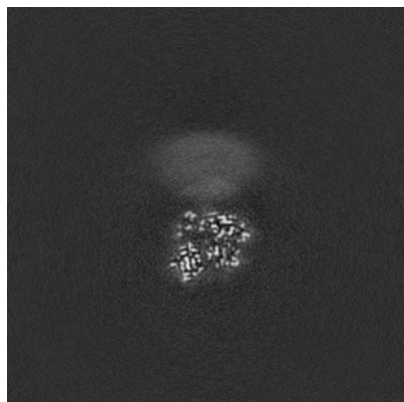


Y Index: 160

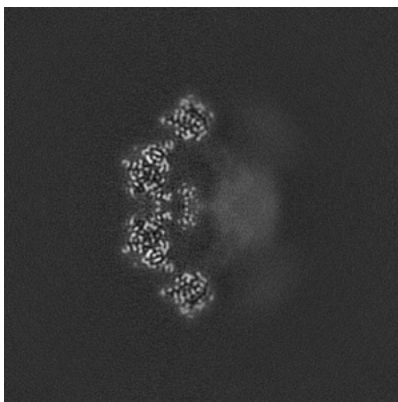


Z Index: 120

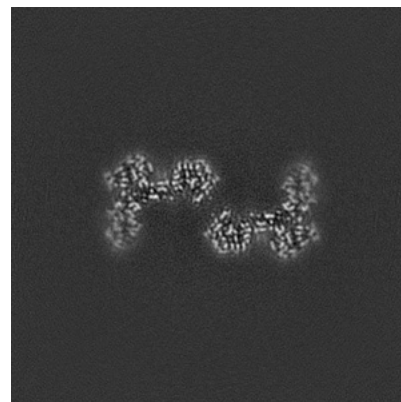
6.3.2 Raw map



X Index: 156



Y Index: 160

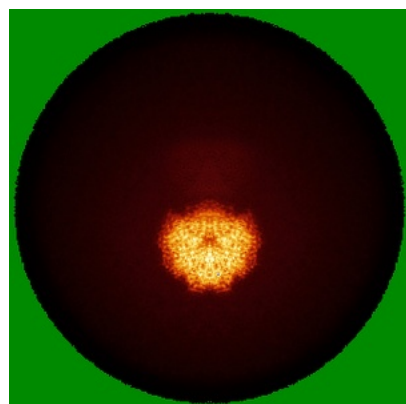


Z Index: 138

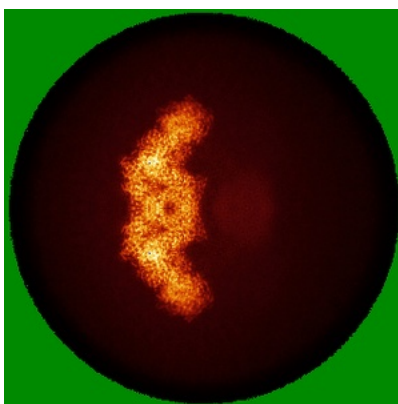
The images above show the largest variance slices of the map in three orthogonal directions.

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

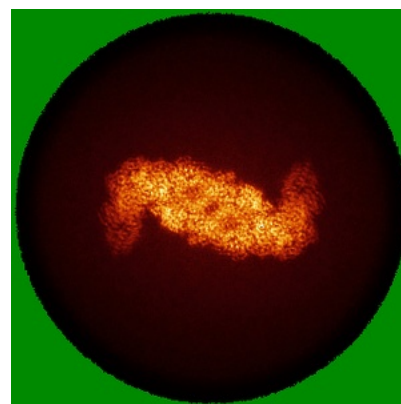
6.4.1 Primary map



X

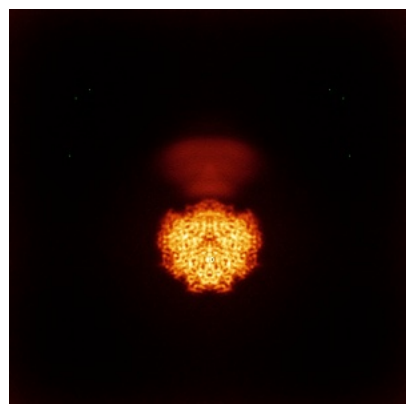


Y

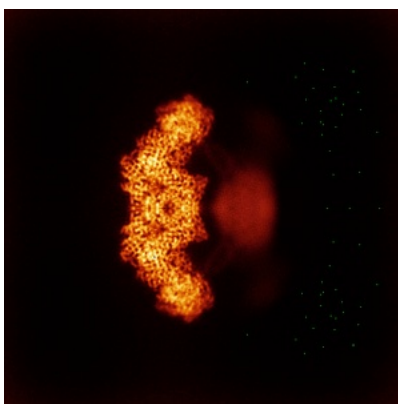


Z

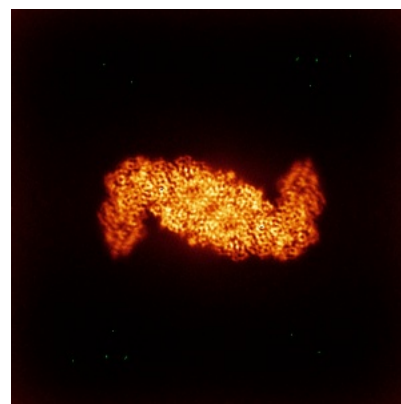
6.4.2 Raw map



X



Y

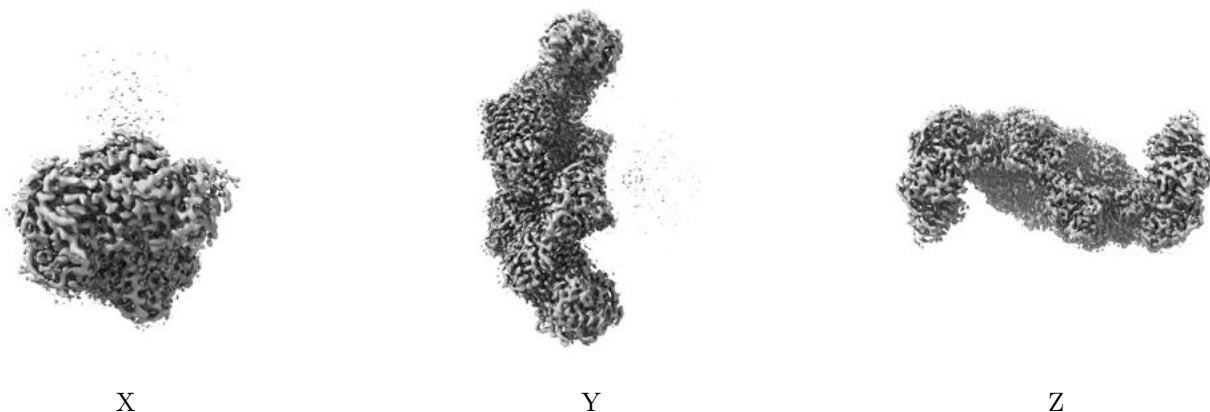


Z

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.

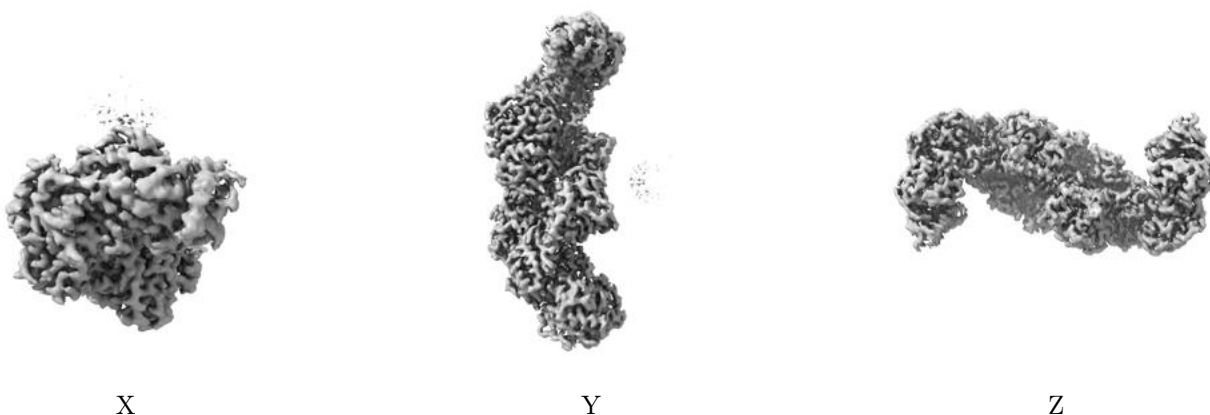
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.286. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

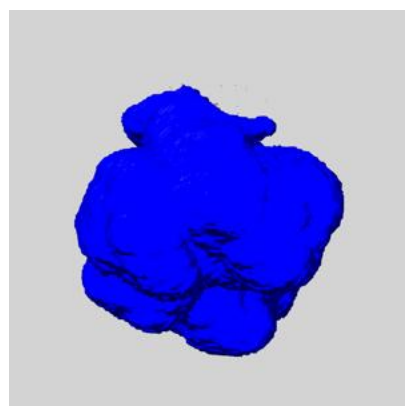
6.6 Mask visualisation [i](#)

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

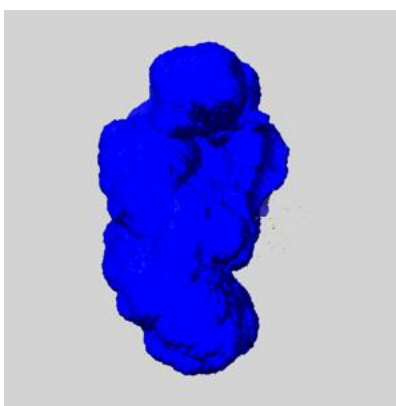
A mask typically either:

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

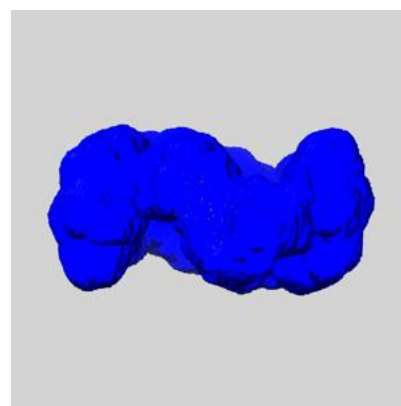
6.6.1 emd_45909_msk_1.map [i](#)



X



Y

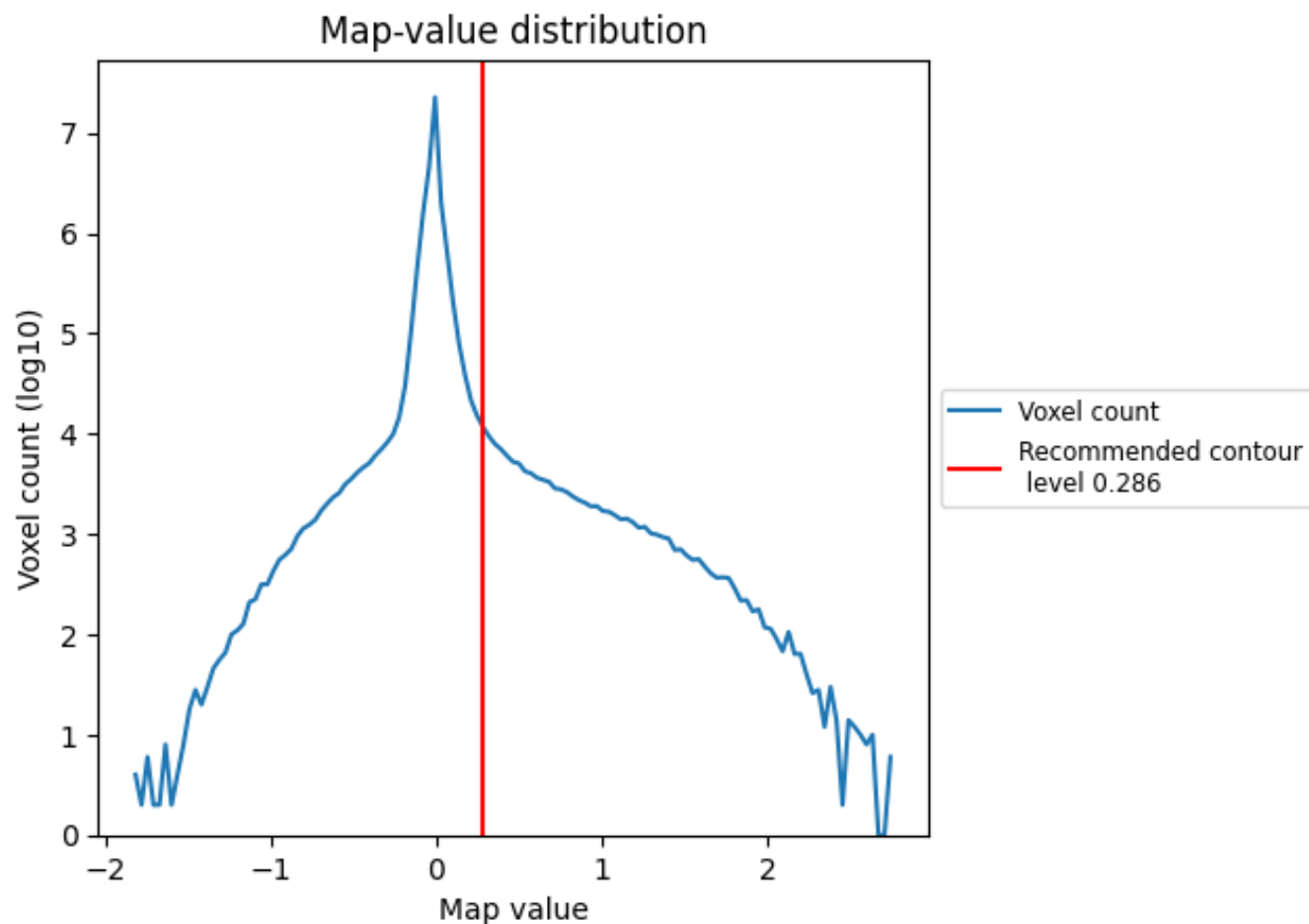


Z

7 Map analysis [i](#)

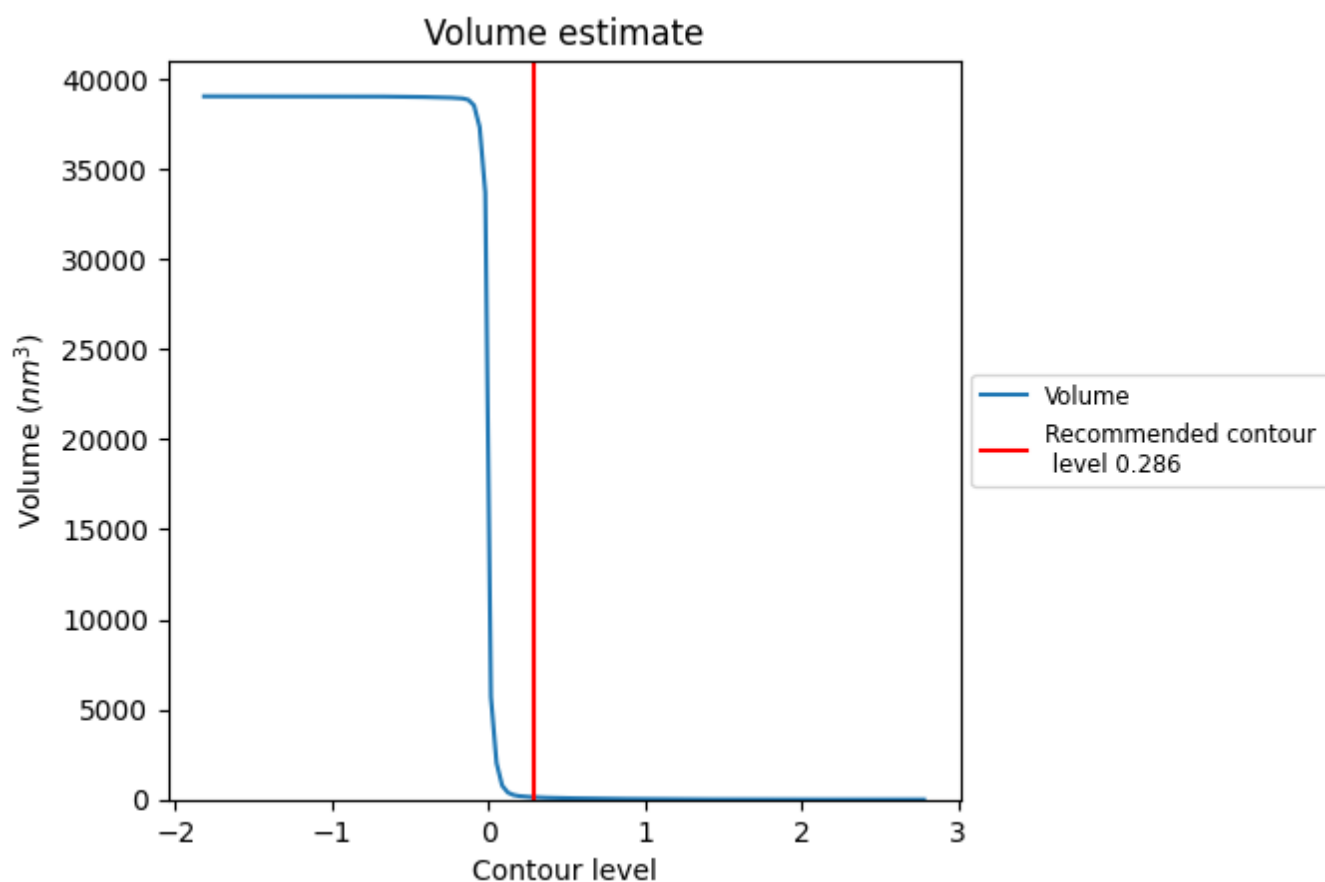
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

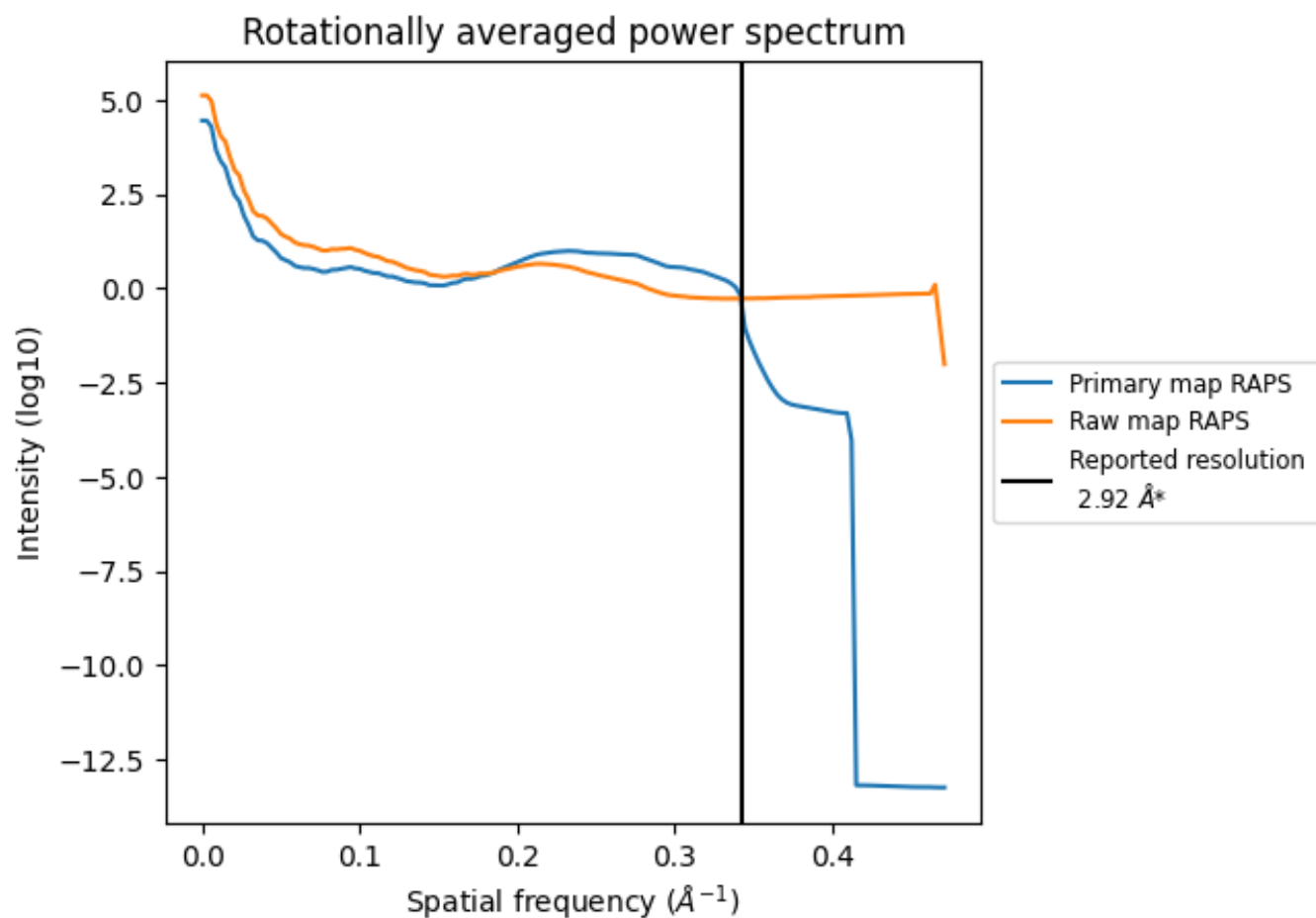
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm³; this corresponds to an approximate mass of 120 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 ⓘ

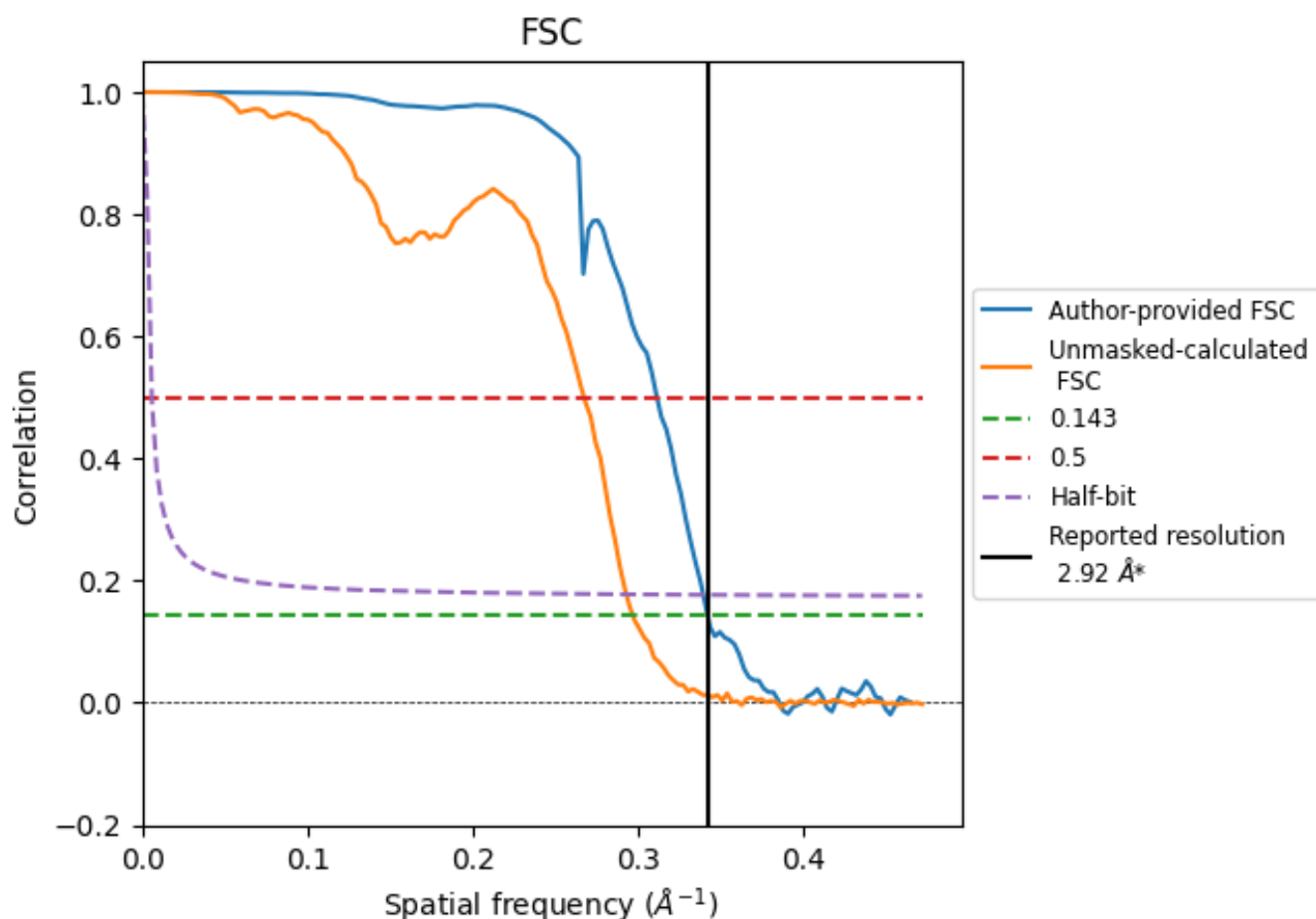


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

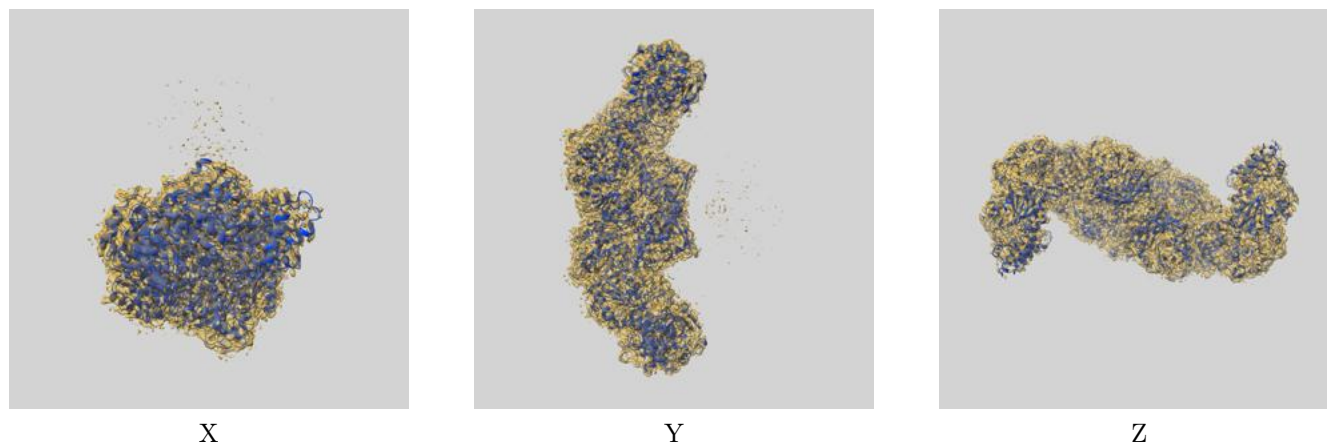
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.21	2.95
Unmasked-calculated*	3.37	3.74	3.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

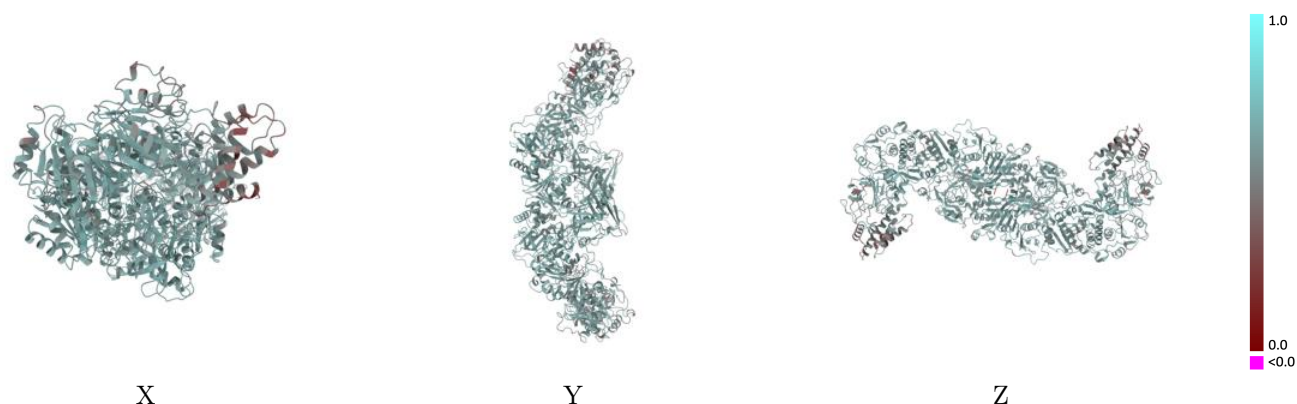
This section contains information regarding the fit between EMDB map EMD-45909 and PDB model 9CTK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



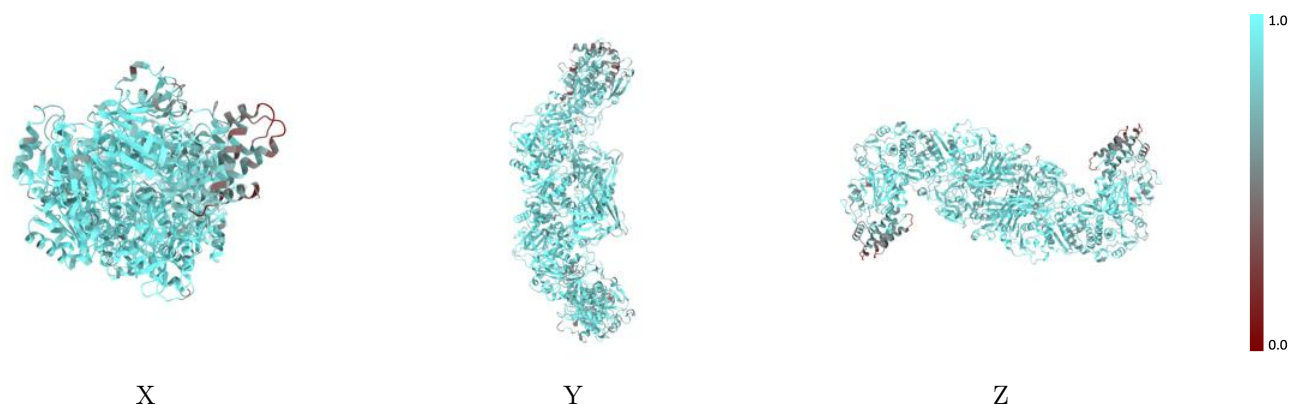
The images above show the 3D surface view of the map at the recommended contour level 0.286 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



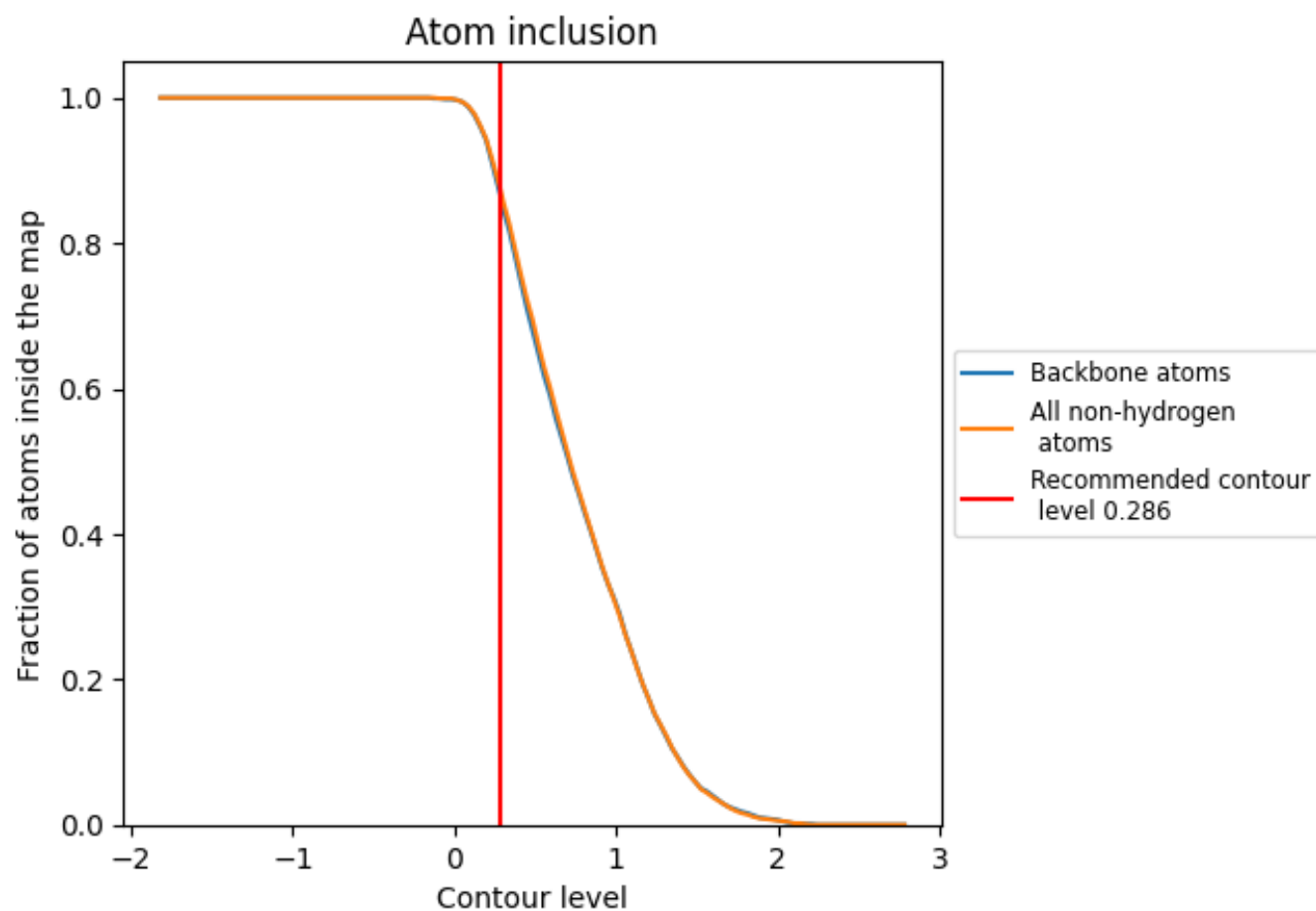
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.286).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.5870
A	0.8750	0.5870
B	0.8750	0.5860

