



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:36 AM UTC

PDB ID : 8T1D / pdb_00008t1d
EMDB ID : EMD-40960
Title : Open-state cryo-EM structure of full-length human TRPV4 in complex with agonist 4a-PDD
Authors : Talyzina, I.A.; Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on : 2023-06-02
Resolution : 3.35 Å(reported)

This is a wwPDB EM Validation Summary 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

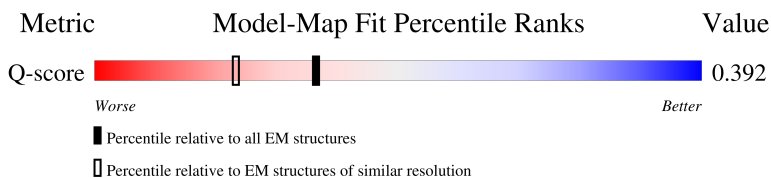
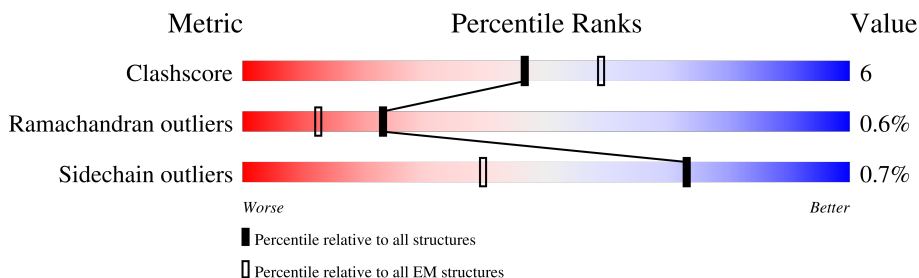
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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	14390 (2.85 - 3.85)

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	1132	14% 46% 9% 44%
1	B	1132	12% 44% 10% 45%
1	C	1132	15% 46% 9% 44%
1	D	1132	13% 44% 10% 45%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 20338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	632	Total	C	N	O	S	0	0
			5086	3309	844	906	27		
1	B	619	Total	C	N	O	S	0	0
			4987	3245	828	889	25		
1	C	632	Total	C	N	O	S	0	0
			5086	3309	844	906	27		
1	D	619	Total	C	N	O	S	0	0
			4987	3245	828	889	25		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	LEU	-	linker	UNP Q9HBA0
A	873	VAL	-	linker	UNP Q9HBA0
A	874	PRO	-	linker	UNP Q9HBA0
A	875	ARG	-	linker	UNP Q9HBA0
A	876	GLY	-	linker	UNP Q9HBA0
A	877	SER	-	linker	UNP Q9HBA0
A	878	ALA	-	linker	UNP Q9HBA0
A	879	ALA	-	linker	UNP Q9HBA0
A	880	ALA	-	linker	UNP Q9HBA0
A	881	ALA	-	linker	UNP Q9HBA0
A	1087	LYS	ALA	engineered mutation	UNP C5MKY7
A	1120	SER	-	expression tag	UNP C5MKY7
A	1121	GLY	-	expression tag	UNP C5MKY7
A	1122	LEU	-	expression tag	UNP C5MKY7
A	1123	ARG	-	expression tag	UNP C5MKY7
A	1124	SER	-	expression tag	UNP C5MKY7
A	1125	TRP	-	expression tag	UNP C5MKY7
A	1126	SER	-	expression tag	UNP C5MKY7
A	1127	HIS	-	expression tag	UNP C5MKY7
A	1128	PRO	-	expression tag	UNP C5MKY7
A	1129	GLN	-	expression tag	UNP C5MKY7

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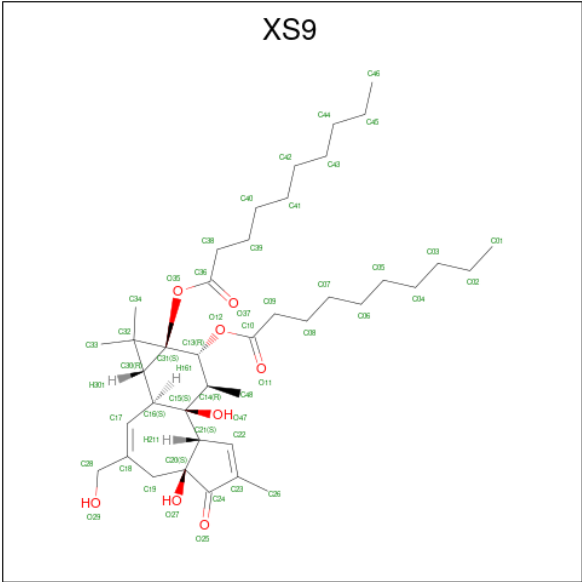
Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	PHE	-	expression tag	UNP C5MKY7
A	1131	GLU	-	expression tag	UNP C5MKY7
A	1132	LYS	-	expression tag	UNP C5MKY7
B	872	LEU	-	linker	UNP Q9HBA0
B	873	VAL	-	linker	UNP Q9HBA0
B	874	PRO	-	linker	UNP Q9HBA0
B	875	ARG	-	linker	UNP Q9HBA0
B	876	GLY	-	linker	UNP Q9HBA0
B	877	SER	-	linker	UNP Q9HBA0
B	878	ALA	-	linker	UNP Q9HBA0
B	879	ALA	-	linker	UNP Q9HBA0
B	880	ALA	-	linker	UNP Q9HBA0
B	881	ALA	-	linker	UNP Q9HBA0
B	1087	LYS	ALA	engineered mutation	UNP C5MKY7
B	1120	SER	-	expression tag	UNP C5MKY7
B	1121	GLY	-	expression tag	UNP C5MKY7
B	1122	LEU	-	expression tag	UNP C5MKY7
B	1123	ARG	-	expression tag	UNP C5MKY7
B	1124	SER	-	expression tag	UNP C5MKY7
B	1125	TRP	-	expression tag	UNP C5MKY7
B	1126	SER	-	expression tag	UNP C5MKY7
B	1127	HIS	-	expression tag	UNP C5MKY7
B	1128	PRO	-	expression tag	UNP C5MKY7
B	1129	GLN	-	expression tag	UNP C5MKY7
B	1130	PHE	-	expression tag	UNP C5MKY7
B	1131	GLU	-	expression tag	UNP C5MKY7
B	1132	LYS	-	expression tag	UNP C5MKY7
C	872	LEU	-	linker	UNP Q9HBA0
C	873	VAL	-	linker	UNP Q9HBA0
C	874	PRO	-	linker	UNP Q9HBA0
C	875	ARG	-	linker	UNP Q9HBA0
C	876	GLY	-	linker	UNP Q9HBA0
C	877	SER	-	linker	UNP Q9HBA0
C	878	ALA	-	linker	UNP Q9HBA0
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C	881	ALA	-	linker	UNP Q9HBA0
C	1087	LYS	ALA	engineered mutation	UNP C5MKY7
C	1120	SER	-	expression tag	UNP C5MKY7
C	1121	GLY	-	expression tag	UNP C5MKY7
C	1122	LEU	-	expression tag	UNP C5MKY7
C	1123	ARG	-	expression tag	UNP C5MKY7

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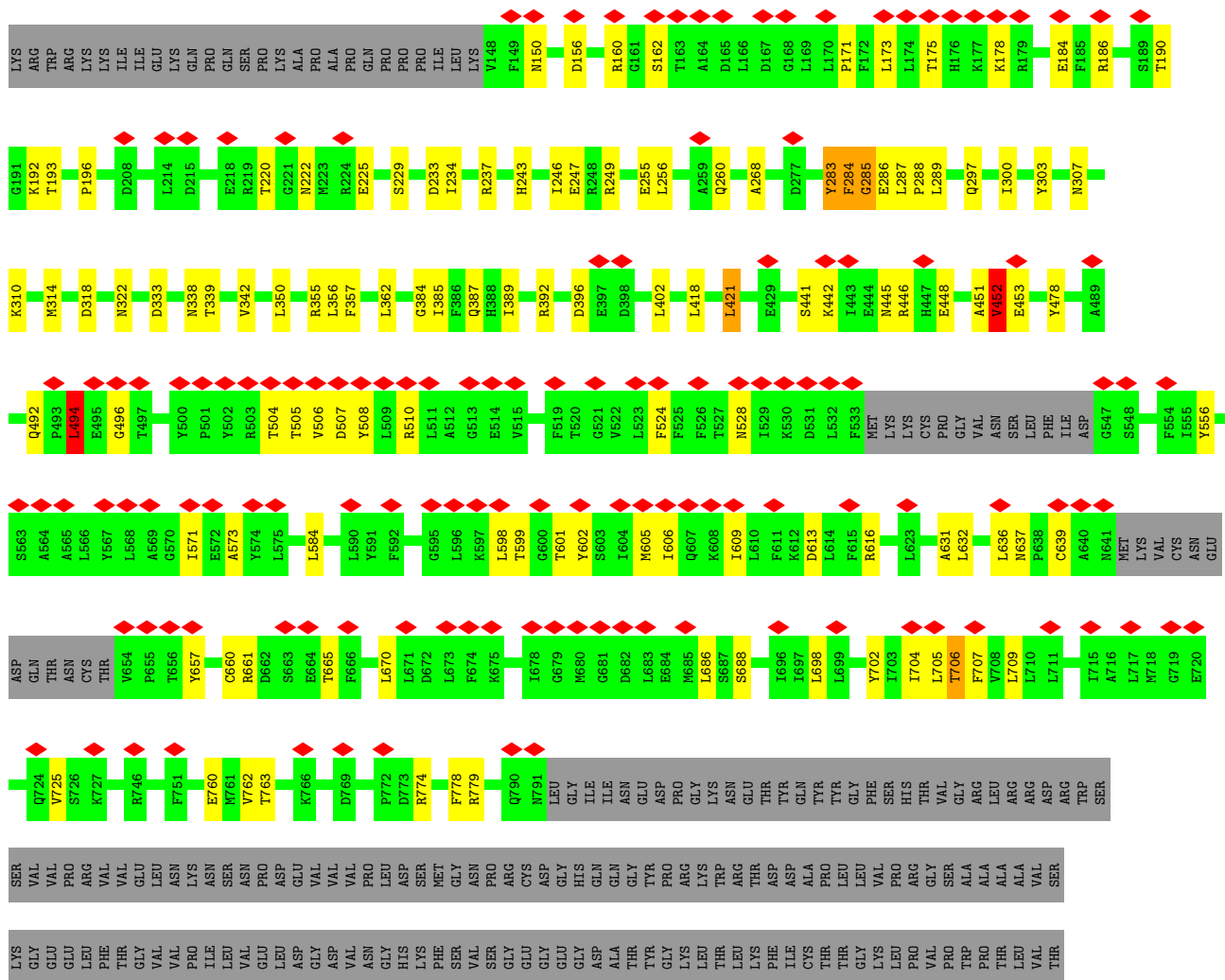
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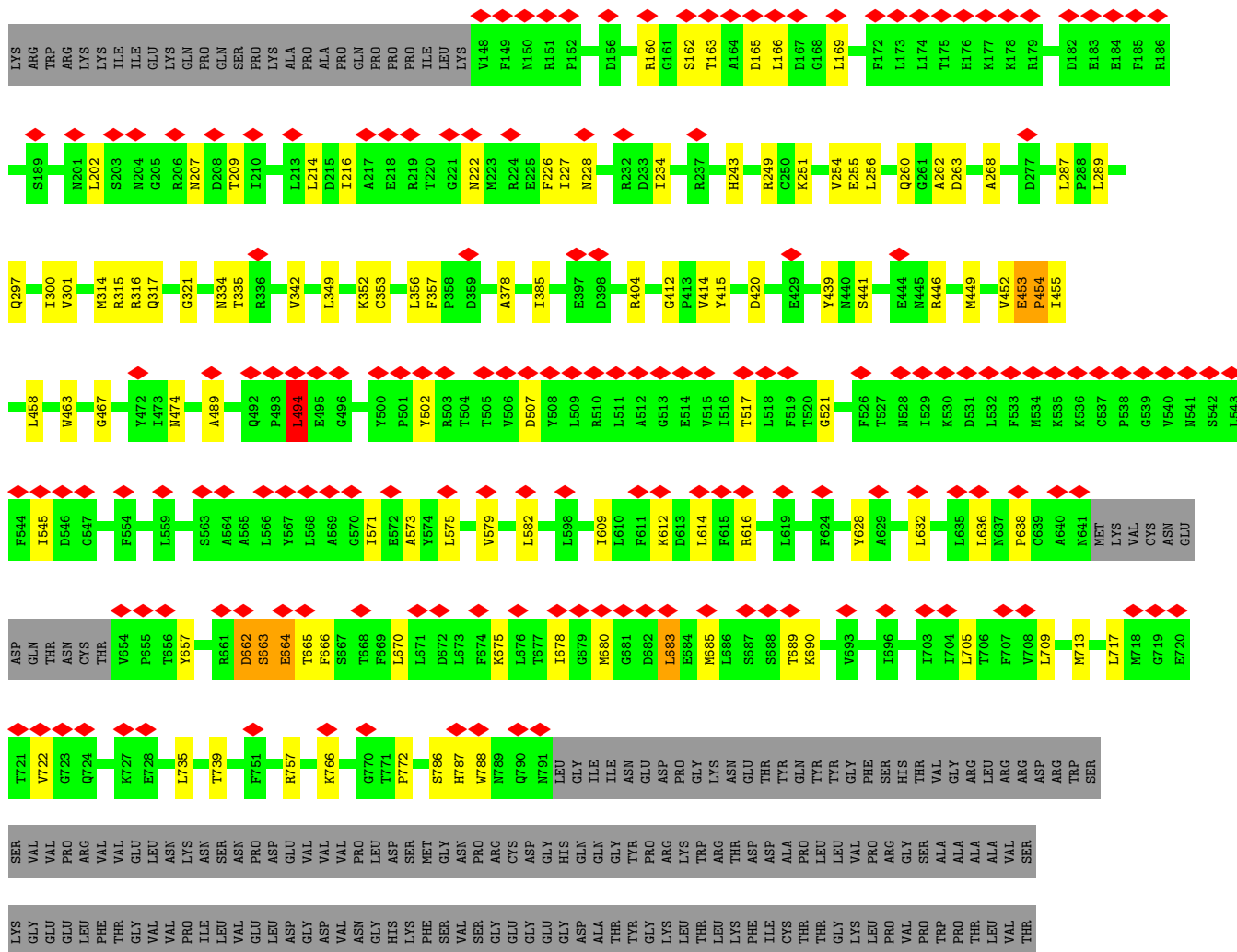
Chain	Residue	Modelled	Actual	Comment	Reference
C	1124	SER	-	expression tag	UNP C5MKY7
C	1125	TRP	-	expression tag	UNP C5MKY7
C	1126	SER	-	expression tag	UNP C5MKY7
C	1127	HIS	-	expression tag	UNP C5MKY7
C	1128	PRO	-	expression tag	UNP C5MKY7
C	1129	GLN	-	expression tag	UNP C5MKY7
C	1130	PHE	-	expression tag	UNP C5MKY7
C	1131	GLU	-	expression tag	UNP C5MKY7
C	1132	LYS	-	expression tag	UNP C5MKY7
D	872	LEU	-	linker	UNP Q9HBA0
D	873	VAL	-	linker	UNP Q9HBA0
D	874	PRO	-	linker	UNP Q9HBA0
D	875	ARG	-	linker	UNP Q9HBA0
D	876	GLY	-	linker	UNP Q9HBA0
D	877	SER	-	linker	UNP Q9HBA0
D	878	ALA	-	linker	UNP Q9HBA0
D	879	ALA	-	linker	UNP Q9HBA0
D	880	ALA	-	linker	UNP Q9HBA0
D	881	ALA	-	linker	UNP Q9HBA0
D	1087	LYS	ALA	engineered mutation	UNP C5MKY7
D	1120	SER	-	expression tag	UNP C5MKY7
D	1121	GLY	-	expression tag	UNP C5MKY7
D	1122	LEU	-	expression tag	UNP C5MKY7
D	1123	ARG	-	expression tag	UNP C5MKY7
D	1124	SER	-	expression tag	UNP C5MKY7
D	1125	TRP	-	expression tag	UNP C5MKY7
D	1126	SER	-	expression tag	UNP C5MKY7
D	1127	HIS	-	expression tag	UNP C5MKY7
D	1128	PRO	-	expression tag	UNP C5MKY7
D	1129	GLN	-	expression tag	UNP C5MKY7
D	1130	PHE	-	expression tag	UNP C5MKY7
D	1131	GLU	-	expression tag	UNP C5MKY7
D	1132	LYS	-	expression tag	UNP C5MKY7

- Molecule 2 is (1aR,1bS,4aS,7aS,7bS,8R,9R,9aS)-9a-(decanoyloxy)-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-1H-cyclopropa[3,4]benzo[1,2-e]azulen-9-yl decanoate (CCD ID: XS9) (formula: C₄₀H₆₄O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			48	40	8	
2	B	1	Total	C	O	0
			48	40	8	
2	C	1	Total	C	O	0
			48	40	8	
2	D	1	Total	C	O	0
			48	40	8	





[illegible]

- Molecule 1: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

[illegible]

F707	F708	L709	L710	L711	F715	A716	L717	M718	G719	E720	G724	S725	S726	K727	E745	R746	F751	E760	M761	T762	T763	K766	D769	G770	R774	F778	R779	Q790	N791	L792	G793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242
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HIS	THR	VAL	GLY	ARG	LEU	ARG	ARG	ASP	TRP	SER	SER	VAL	PRO	VAL	VAL	ASN	LYS	ASN	SER	ASN	PRO	PRO	GLU	GLU	VAL	VAL	ASP	GLU	VAL	VAL	PRO	LEU	ASP	SER	MET	GLY	ASN	ASN	PRO	GLN	GLN	GLY	TYP	THR	PRO	PRO	LEU					
LEU	VAL	PRO	ARG	GLY	SER	ALA	ALA	ALA	ALA	SER	LYS	GLY	GLU	GLU	PHE	THR	VAL	LEU	ILE	LEU	VAL	GLU	LEU	ASP	GLY	ASP	VAL	VAL	ASN	GLY	HIS	LYS	PHE	SER	VAL	ASP	GLY	ALA	ALA	THR	TYP	GLY	LYS	LEU	THR	LEU	LYS	PHE	ILE	CYS	THR	THR

GLY	GLU	ILE
LYS	VAL	GLU
LEU	LYS	ASP
PRO	PHE	GLY
VAL	GLU	SER
PRO	GLY	VAL
TRP	ASP	GLN
PRO	THR	LEU
THR	LEU	ALA
VAL	VAL	ASP
ASN	ARG	HIS
THR	ILE	TYR
THR	GLU	GLN
LEU	LEU	ASN
THR	LYS	THR
TYR	GLY	PRO
GLY	ILE	ILE
VAL	ASP	GLY
GLN	PHE	ASP
CYS	LYS	GLY
PHE	GLU	PRO
SER	ASP	VAL
ARG	GLY	VAL
TYR	ASN	LEU
PRO	ILE	LEU
ASP	ILE	PRO
HIS	LEU	ASP
MET	GLY	ASN
LYS	HIS	HIS
GLN	LYS	TYR
LYS	LEU	SER
HIS	GLU	THR
ASP	PHE	GLN
PHE	ASN	SER
LYS	TYR	LYS
SER	ASN	LEU
ALA	SER	SER
MET	HIS	SER
PRO	ASN	LYS
GLU	VAL	ASP
TYR	TYR	PRO
ILE	ILE	ASN
TYR	MET	GLU
VAL	ALA	LYS
GLN	ASP	ARG
GLU	ARG	ASP
THR	LYS	HIS
THR	GLN	THR
ILE	LYS	MET
PHE	ASN	VAL
PHE	GLY	LEU
LYS	ILE	LEU
ASP	LYS	GLU
GLY	VAL	PHE
ASN	ASN	THR
ASN	PHE	ALA
TYR	LYS	ALA
LYS	ILE	GLY
THR	ARG	ILE
ARG	HIS	THR
ALA	ASN	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.323	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	252.416, 252.416, 252.416	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.7888, 0.7888, 0.7888	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XS9

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	0.31	1/5206 (0.0%)	0.84	8/7061 (0.1%)
1	B	0.30	0/5104	0.79	5/6923 (0.1%)
1	C	0.31	1/5206 (0.0%)	0.84	8/7061 (0.1%)
1	D	0.30	0/5104	0.79	5/6923 (0.1%)
All	All	0.31	2/20620 (0.0%)	0.82	26/27968 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	657	TYR	C-N	6.39	1.40	1.34
1	A	657	TYR	C-N	6.38	1.40	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	SER	CA-C-N	7.87	136.57	121.54
1	A	663	SER	C-N-CA	7.87	136.57	121.54
1	C	663	SER	CA-C-N	7.86	136.55	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	663	SER	C-N-CA	7.86	136.55	121.54
1	C	662	ASP	CA-C-N	6.49	133.93	121.54

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ASN	Peptide
1	A	453	GLU	Peptide
1	A	662	ASP	Peptide
1	A	664	GLU	Peptide
1	A	680	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5086	0	5148	61	0
1	B	4987	0	5042	69	0
1	C	5086	0	5148	61	0
1	D	4987	0	5042	72	0
2	A	48	0	0	2	0
2	B	48	0	0	3	0
2	C	48	0	0	2	0
2	D	48	0	0	3	0
All	All	20338	0	20380	247	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.

The worst 5 of 247 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:D:441:SER:HB3	1:D:446:ARG:HE	1.55	0.72
1:B:441:SER:HB3	1:B:446:ARG:HE	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ARG:HG3	1:C:420:ASP:HB3	1.76	0.68
1:A:404:ARG:HG3	1:A:420:ASP:HB3	1.76	0.67
1:B:494:LEU:HD13	1:B:496:GLY:H	1.62	0.65

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	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	21	49
1	B	613/1132 (54%)	553 (90%)	56 (9%)	4 (1%)	18	46
1	C	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	21	49
1	D	613/1132 (54%)	552 (90%)	57 (9%)	4 (1%)	18	46
All	All	2482/4528 (55%)	2163 (87%)	303 (12%)	16 (1%)	23	49

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	SER
1	A	665	THR
1	C	663	SER
1	C	665	THR
1	A	335	THR

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	558/987 (56%)	556 (100%)	2 (0%)	84	82
1	B	546/987 (55%)	540 (99%)	6 (1%)	65	73
1	C	558/987 (56%)	556 (100%)	2 (0%)	84	82
1	D	546/987 (55%)	540 (99%)	6 (1%)	65	73
All	All	2208/3948 (56%)	2192 (99%)	16 (1%)	73	77

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	670	LEU
1	D	494	LEU
1	C	494	LEU
1	D	421	LEU
1	B	686	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	150	ASN
1	D	361	ASN
1	D	228	ASN
1	D	297	GLN
1	D	456	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	XS9	B	1201	-	46,51,51	0.53	1 (2%)	39,76,76	0.68	2 (5%)
2	XS9	C	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	A	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	D	1201	-	46,51,51	0.53	1 (2%)	39,76,76	0.68	2 (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	XS9	B	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	C	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	A	1201	-	-	14/29/108/108	0/4/4/4
2	XS9	D	1201	-	-	15/29/108/108	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	XS9	C15-C14	-2.88	1.49	1.55
2	D	1201	XS9	C15-C14	-2.86	1.49	1.55

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	XS9	C48-C14-C15	4.64	118.59	113.34
2	A	1201	XS9	C48-C14-C15	4.61	118.56	113.34
2	A	1201	XS9	C31-O35-C36	3.69	128.15	119.93
2	C	1201	XS9	C31-O35-C36	3.68	128.13	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	1201	XS9	C31-O35-C36	3.11	126.86	119.93

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

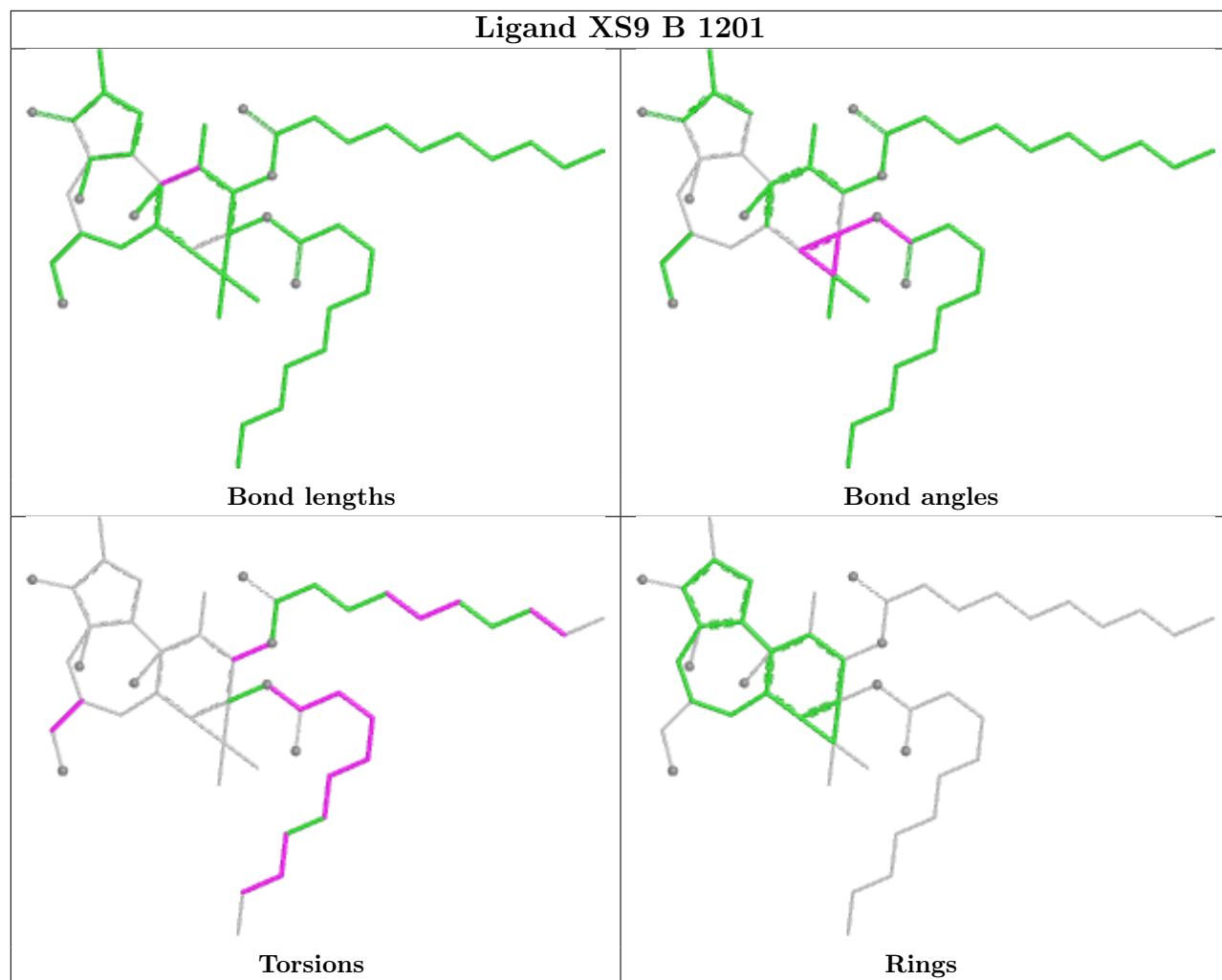
Mol	Chain	Res	Type	Atoms
2	A	1201	XS9	C17-C18-C28-O29
2	A	1201	XS9	C19-C18-C28-O29
2	A	1201	XS9	O37-C36-O35-C31
2	A	1201	XS9	C38-C36-O35-C31
2	B	1201	XS9	C17-C18-C28-O29

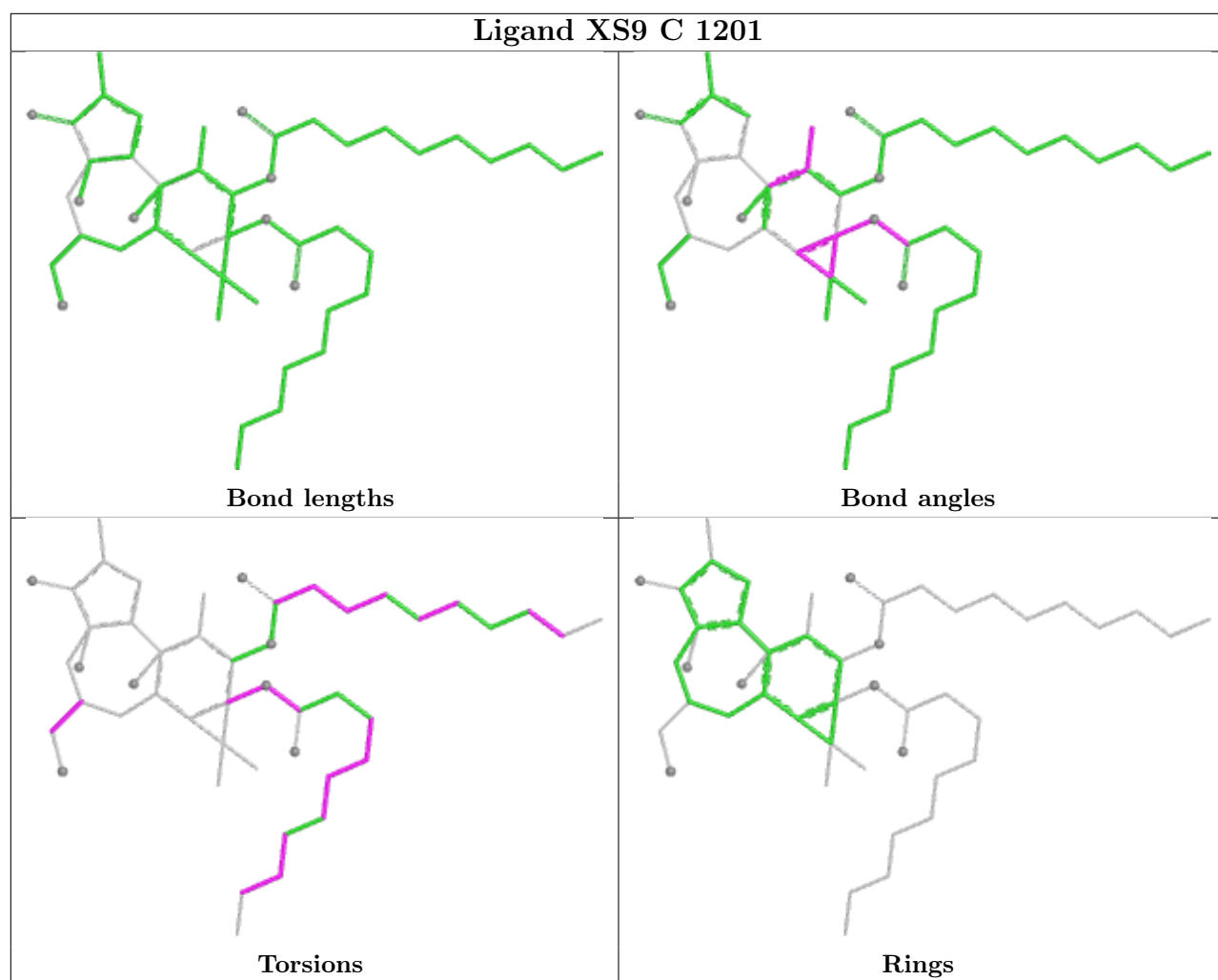
There are no ring outliers.

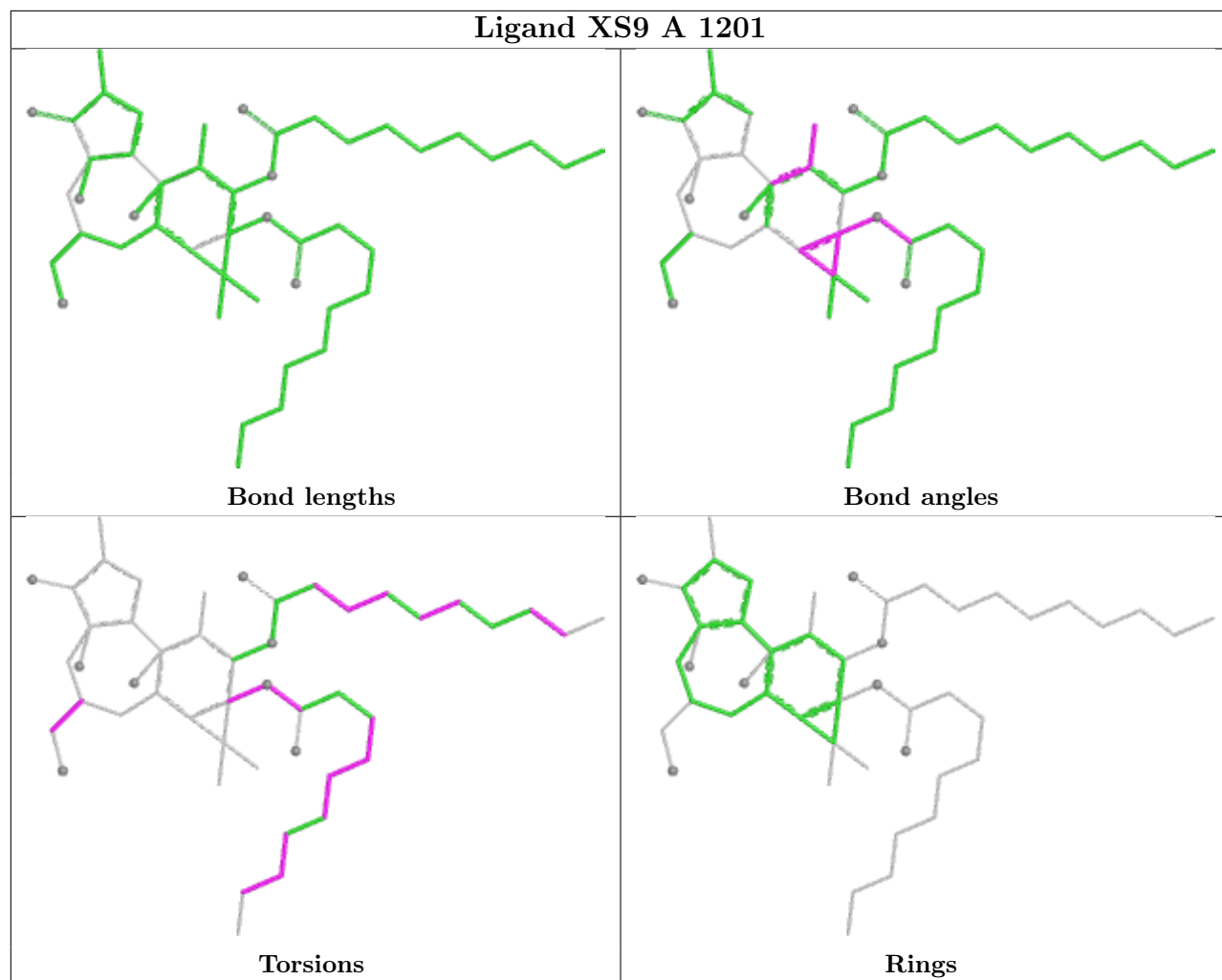
4 monomers are involved in 10 short contacts:

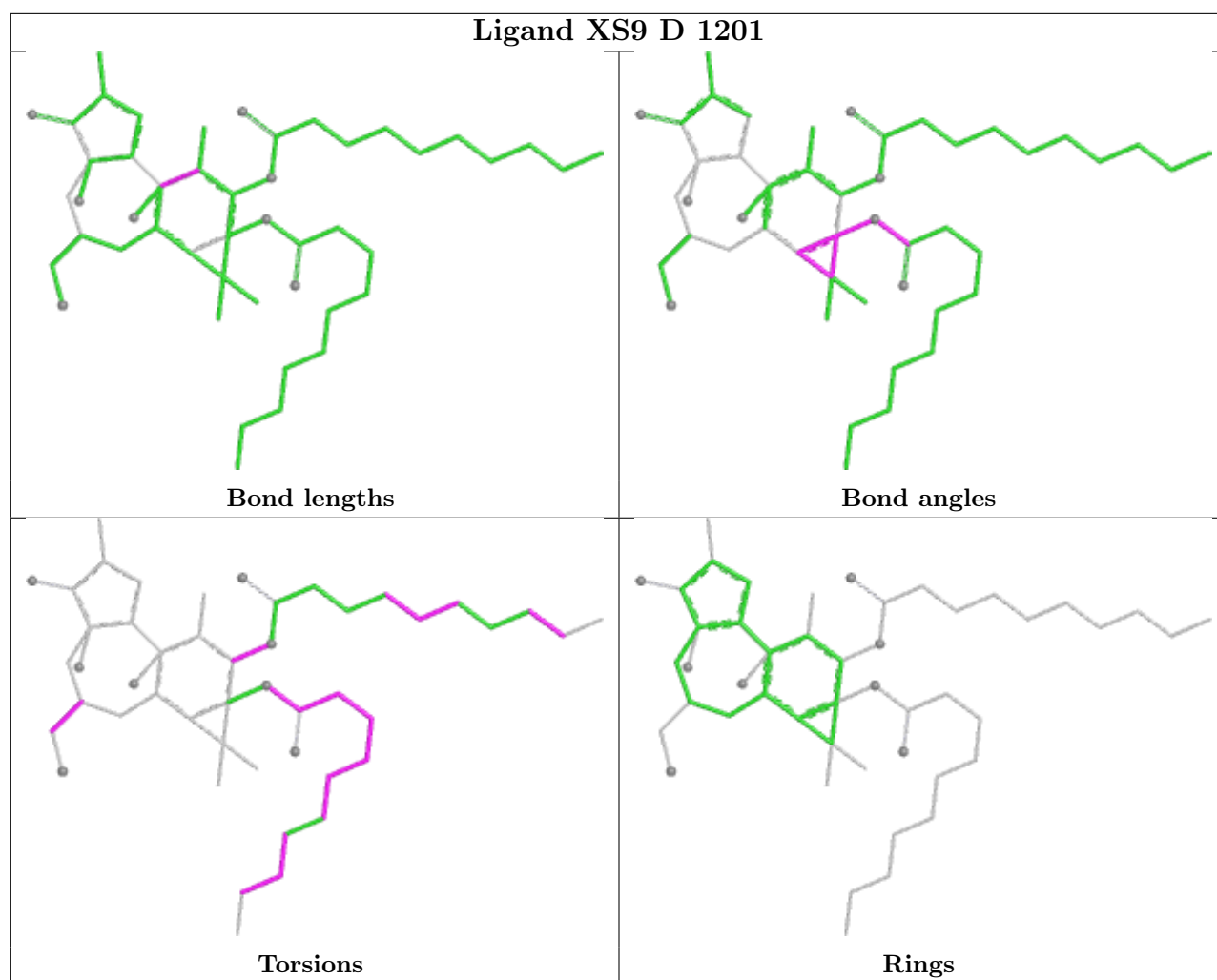
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	XS9	3	0
2	C	1201	XS9	2	0
2	A	1201	XS9	2	0
2	D	1201	XS9	3	0

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.

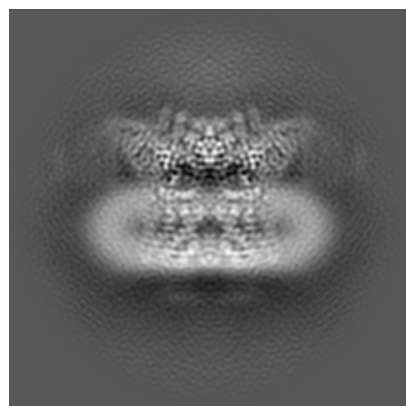
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40960. These allow visual inspection of the internal detail of the map and identification of artifacts.

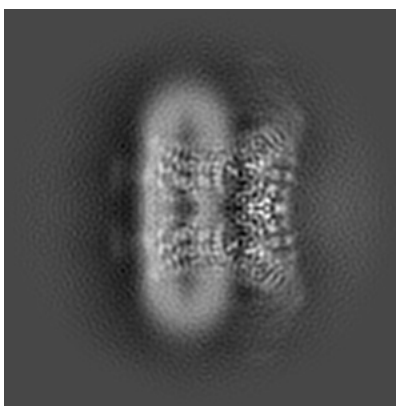
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

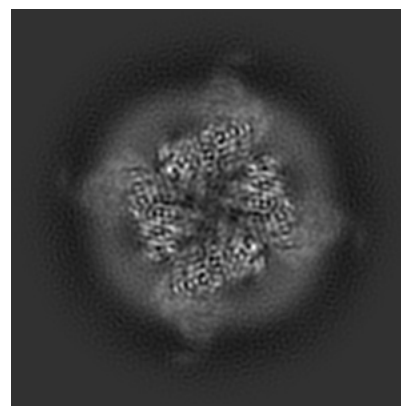
6.1.1 Primary map



X

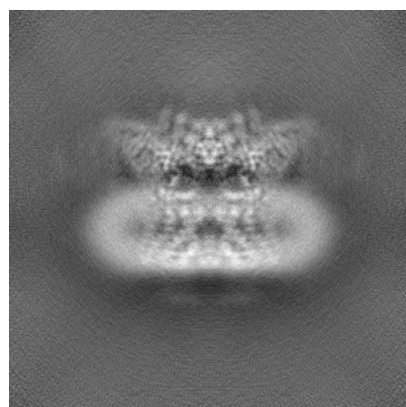


Y

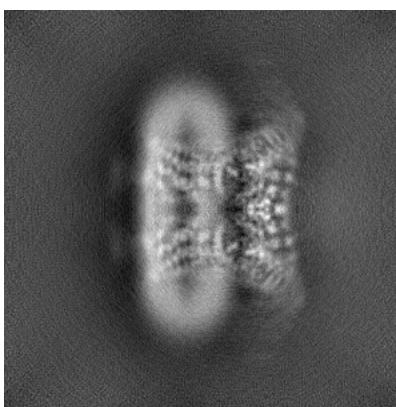


Z

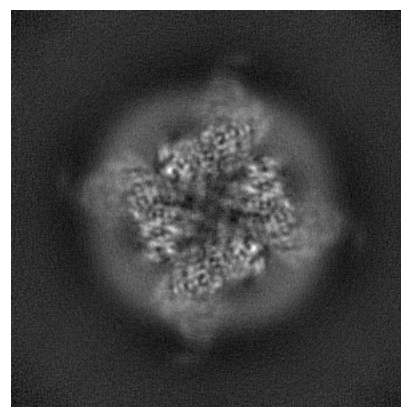
6.1.2 Raw map



X



Y



Z

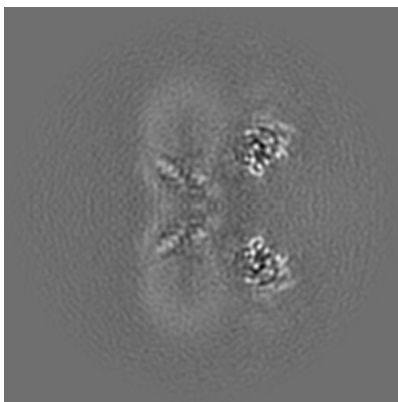
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

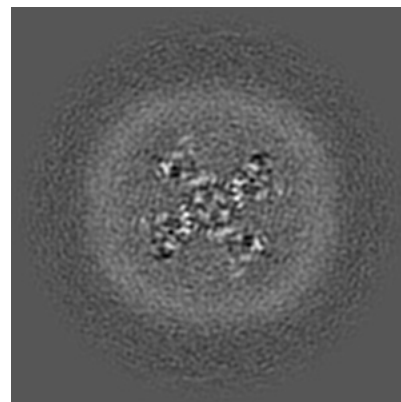
6.2.1 Primary map



X Index: 160

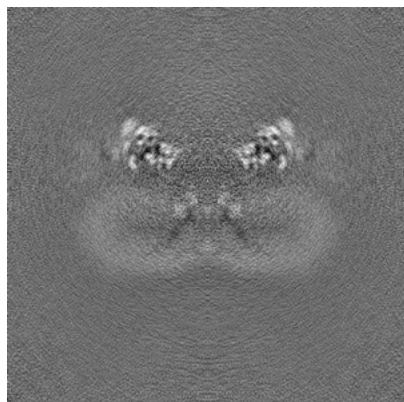


Y Index: 160

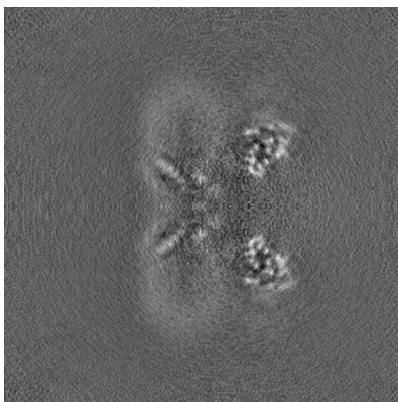


Z Index: 160

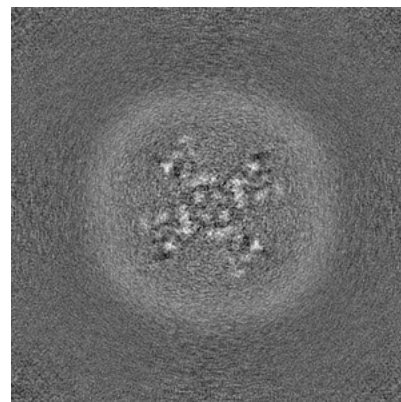
6.2.2 Raw map



X Index: 160



Y Index: 160

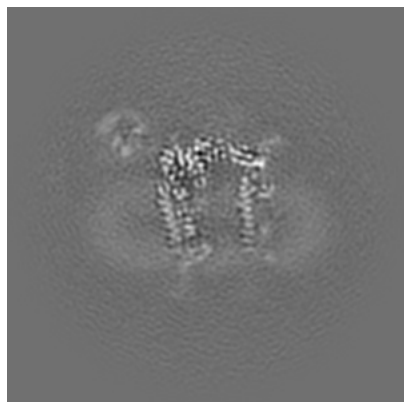


Z Index: 160

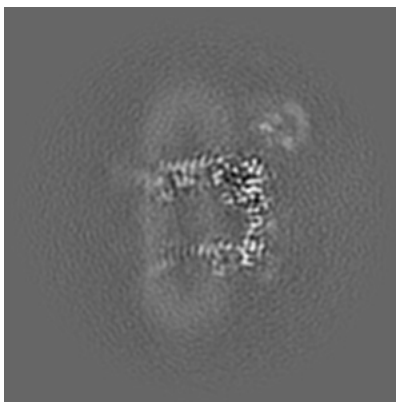
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

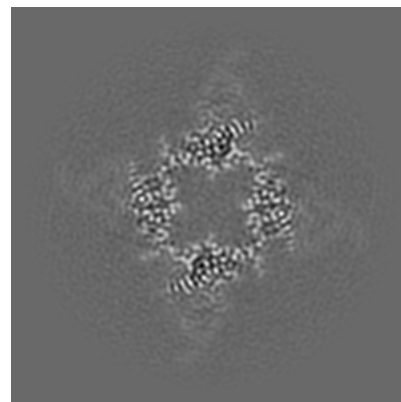
6.3.1 Primary map



X Index: 125

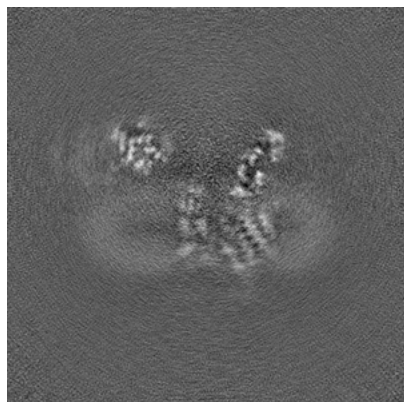


Y Index: 126

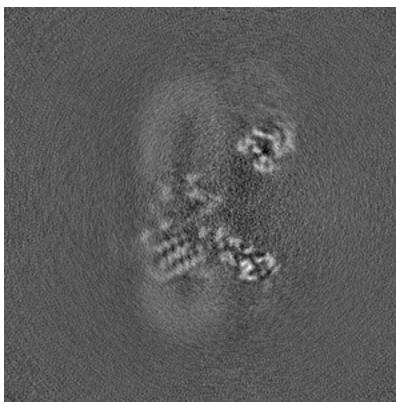


Z Index: 205

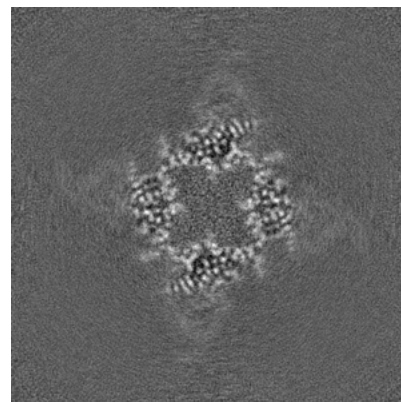
6.3.2 Raw map



X Index: 142



Y Index: 148

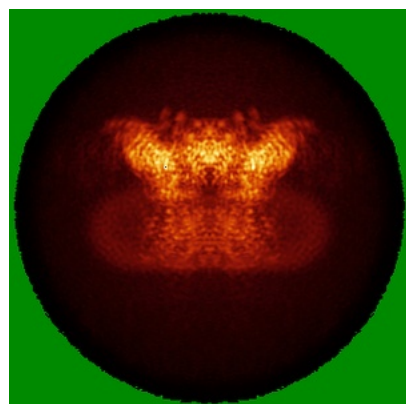


Z Index: 205

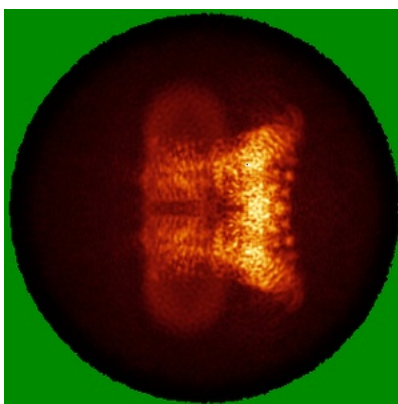
The images above show the largest variance slices of the map in three orthogonal directions.

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

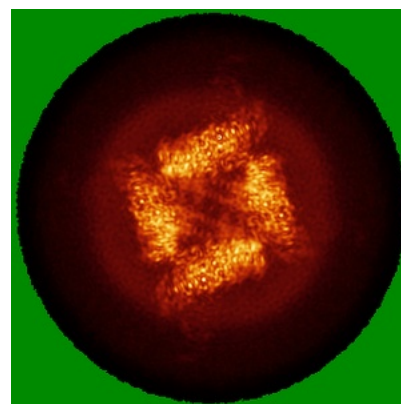
6.4.1 Primary map



X

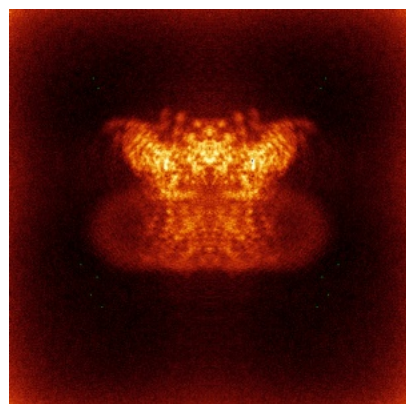


Y

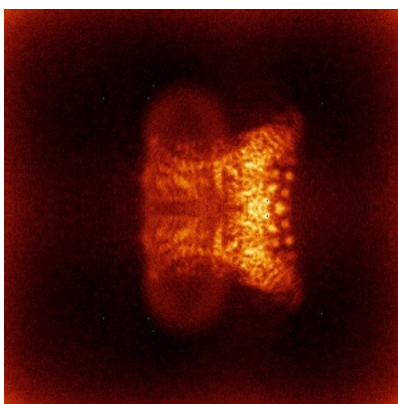


Z

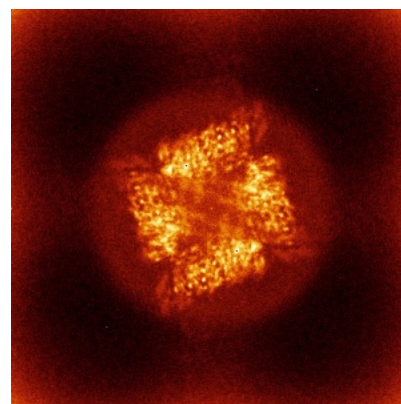
6.4.2 Raw map



X



Y

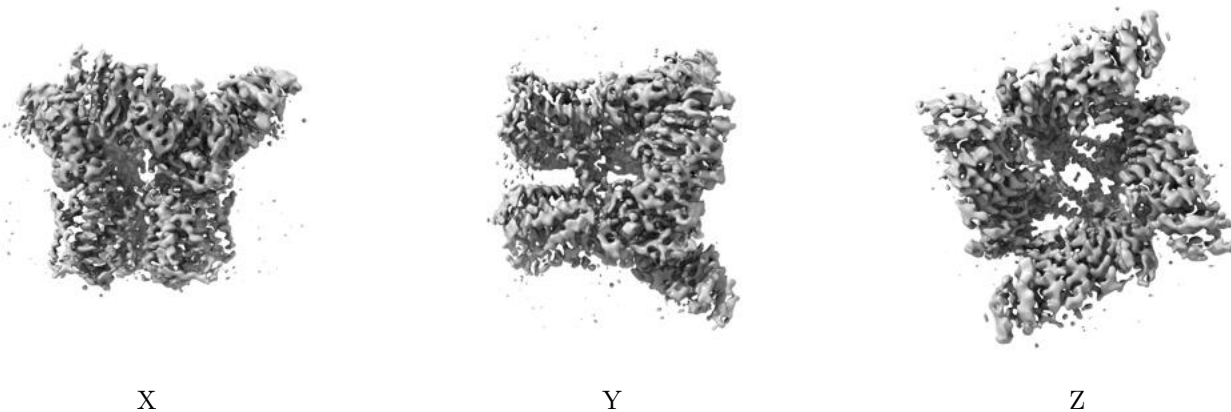


Z

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.

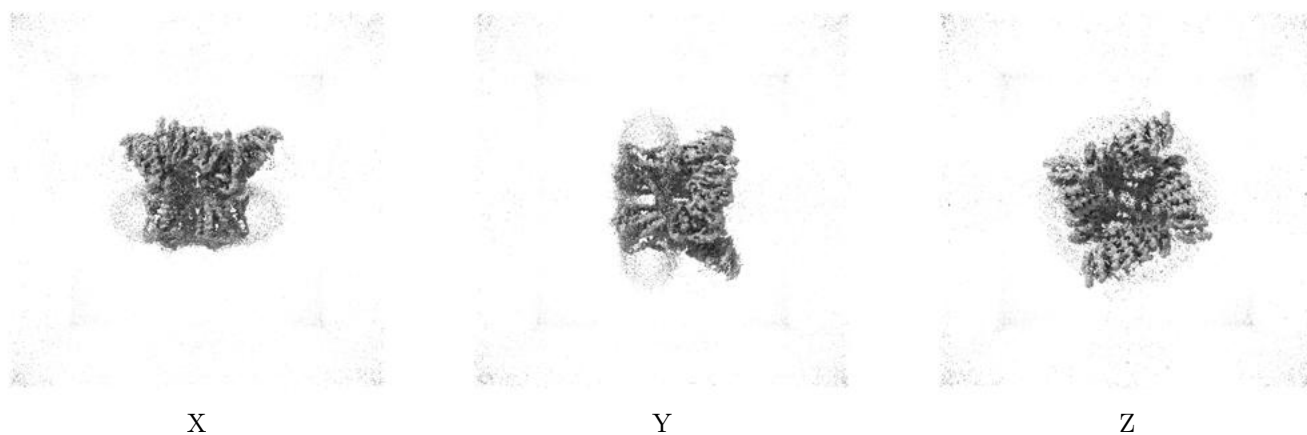
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

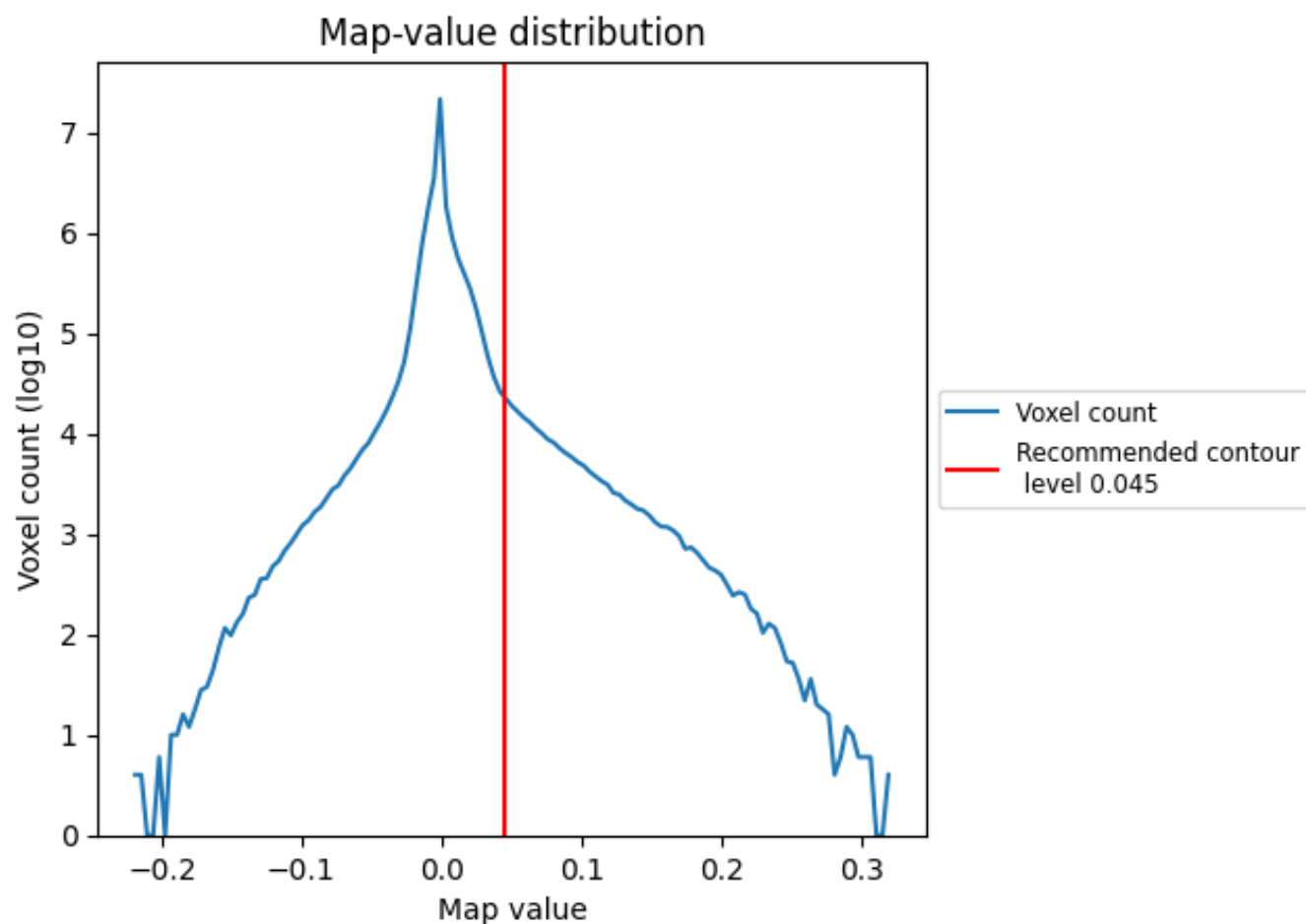
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

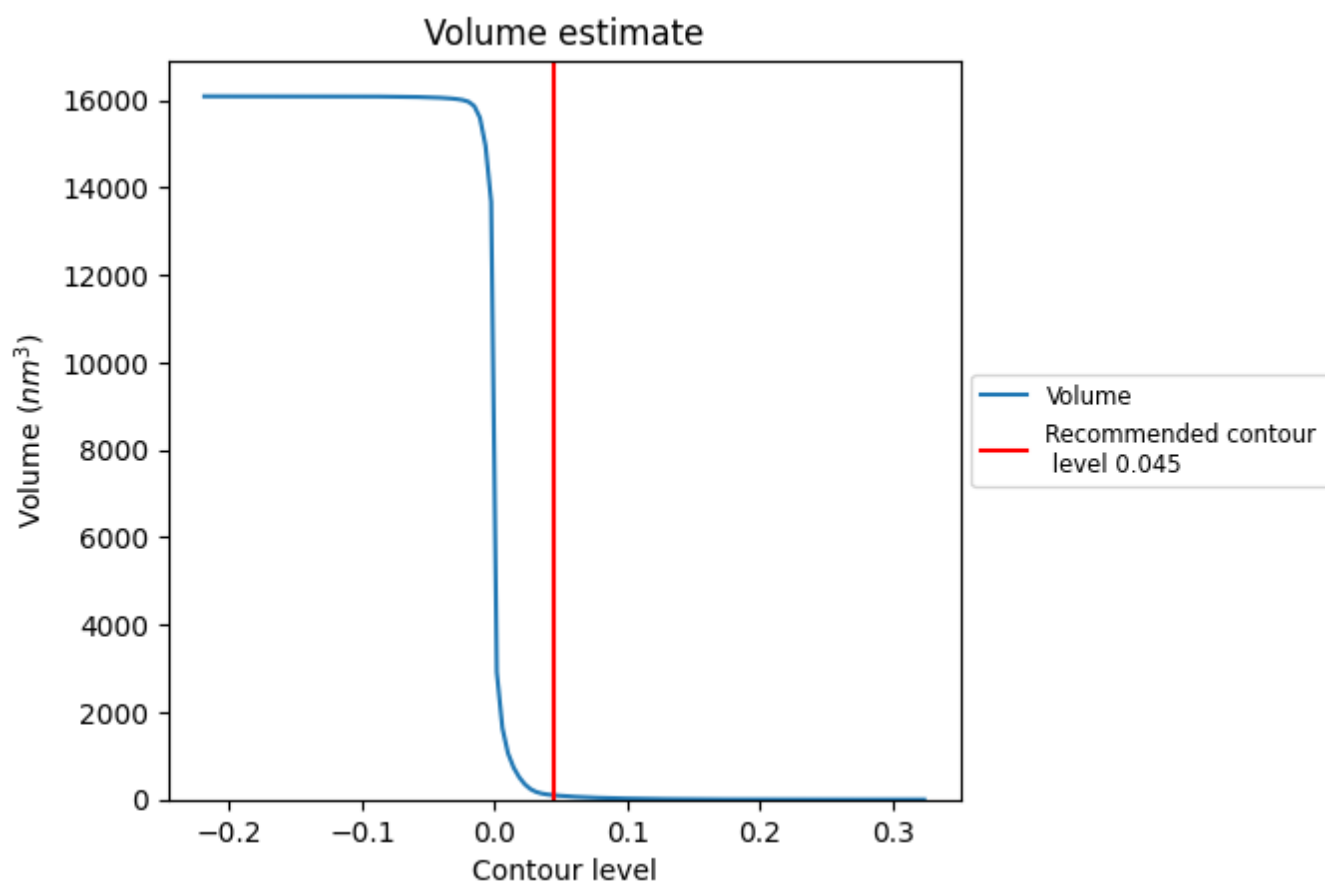
This section contains the results of statistical analysis of the map.

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.

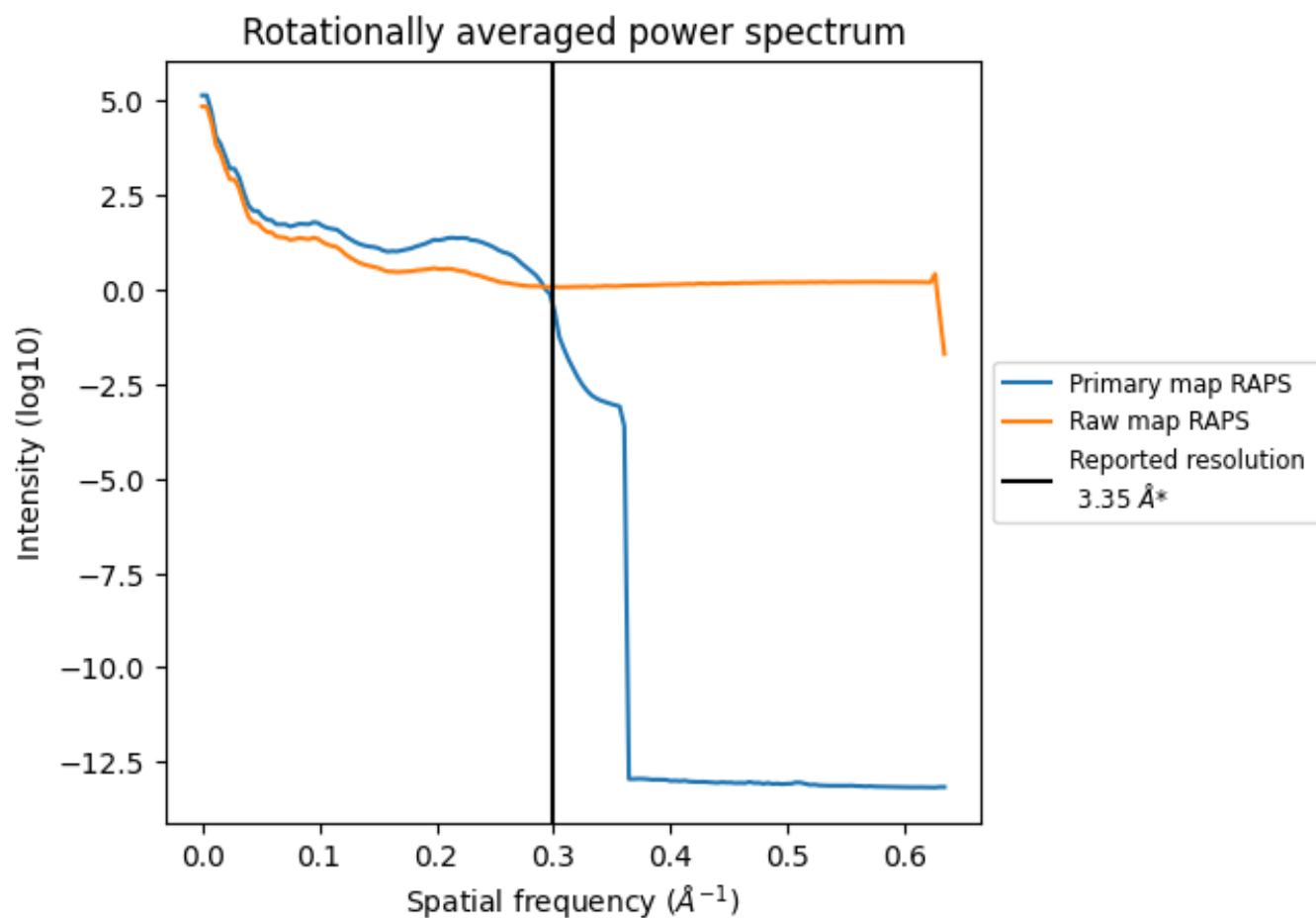
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

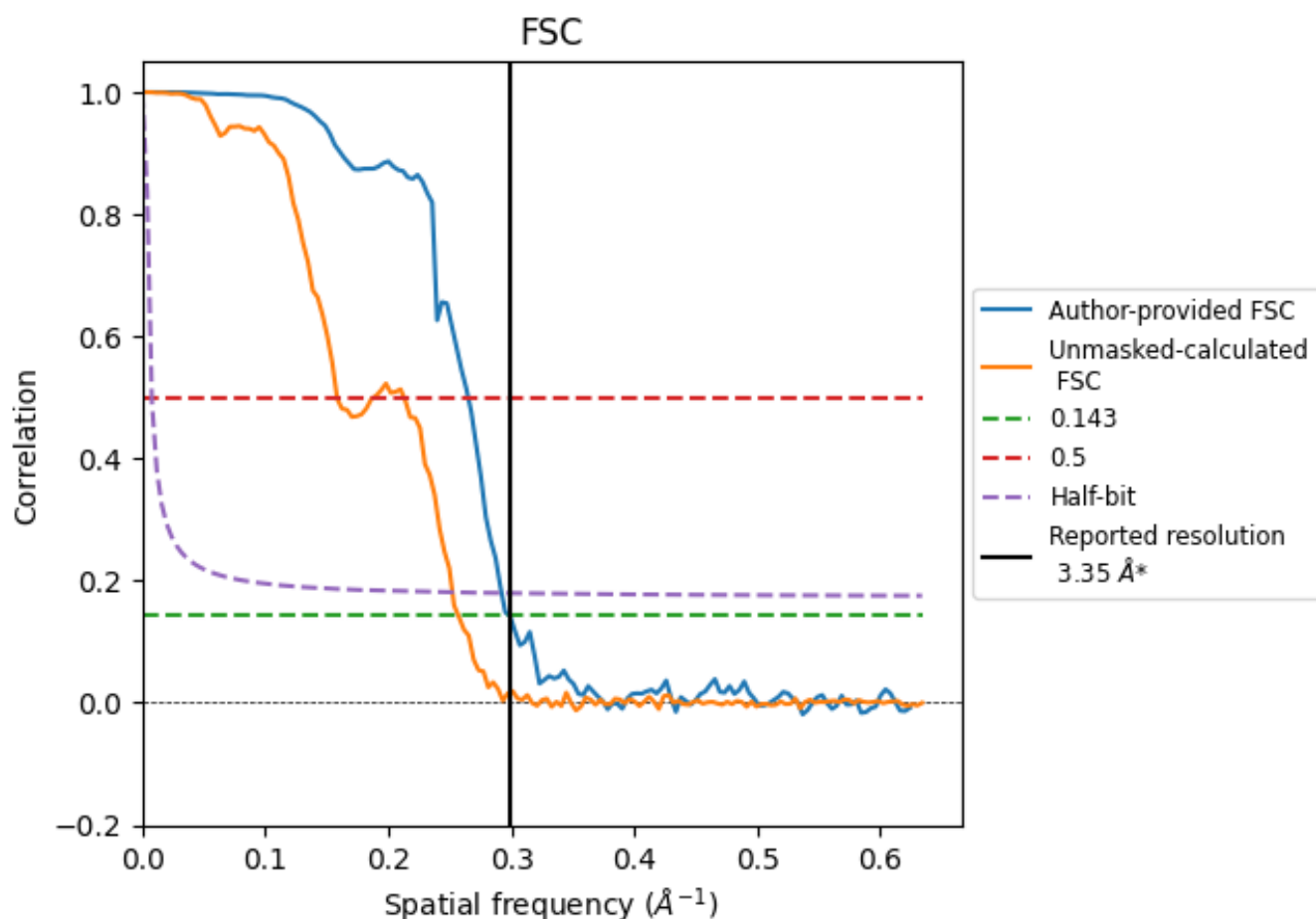


*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

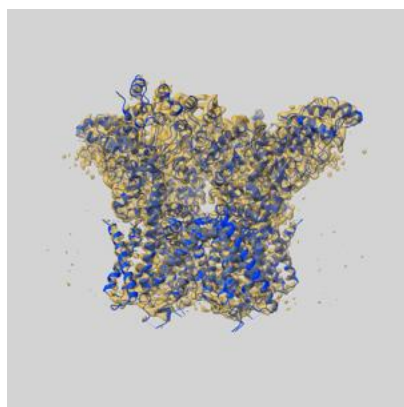
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.42
Unmasked-calculated*	3.89	6.32	3.97

*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 3.89 differs from the reported value 3.35 by more than 10 %

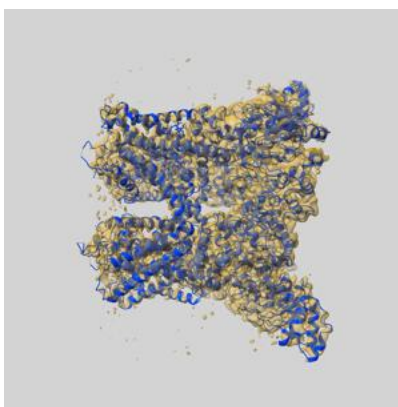
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40960 and PDB model 8T1D. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

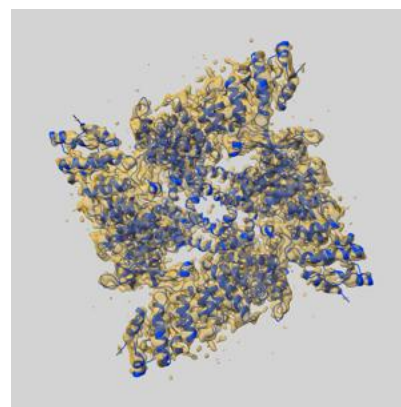
9.1 Map-model overlay [i](#)



X



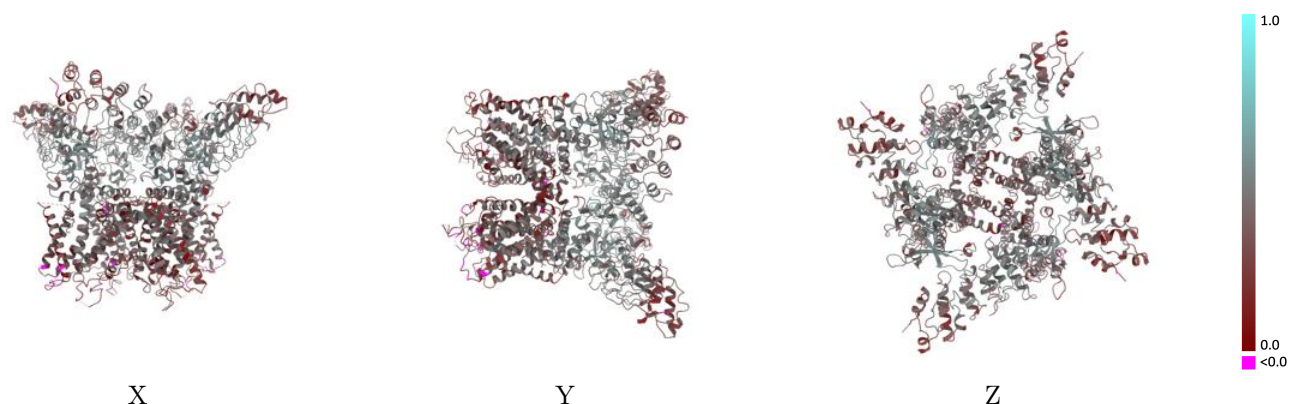
Y



Z

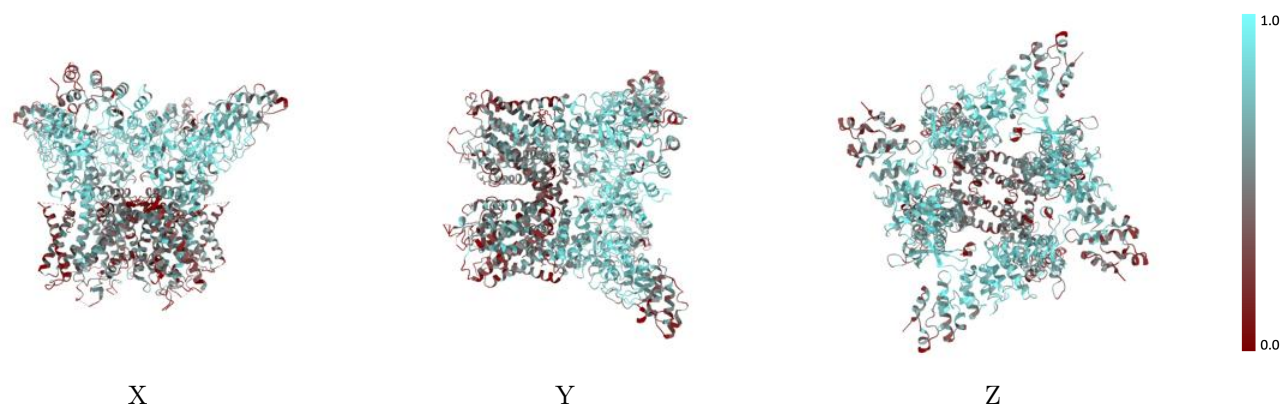
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



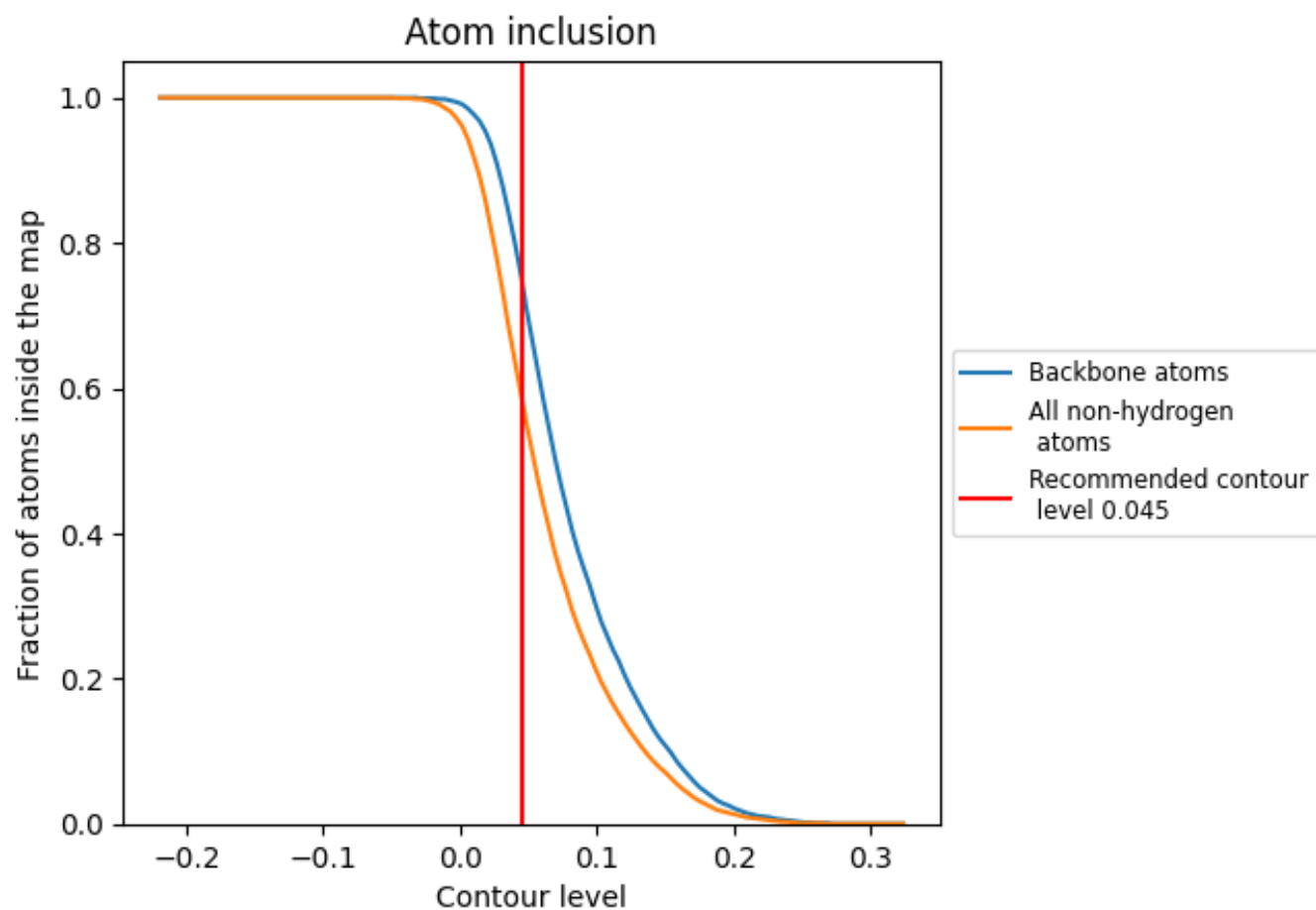
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 59% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5880	0.3920
A	0.5780	0.3940
B	0.6060	0.3990
C	0.5720	0.3880
D	0.5970	0.3880

