wwPDB EM Validation Summary Report

Sep 16, 2026 – 05:24 PM EDT

PDB ID	:	9DFS / pdb_00009dfs
EMDB ID	:	EMD-46818
Title	:	Structure of novel Myo7a-N isoform (ADP-bound) expressed in sensory hair cells (head domain + first two IQ domains), bound to F-actin
Authors	:	Egelman, E.H.; Shin, J.B.
Deposited on	:	2024-08-30
Resolution	:	3.10 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:

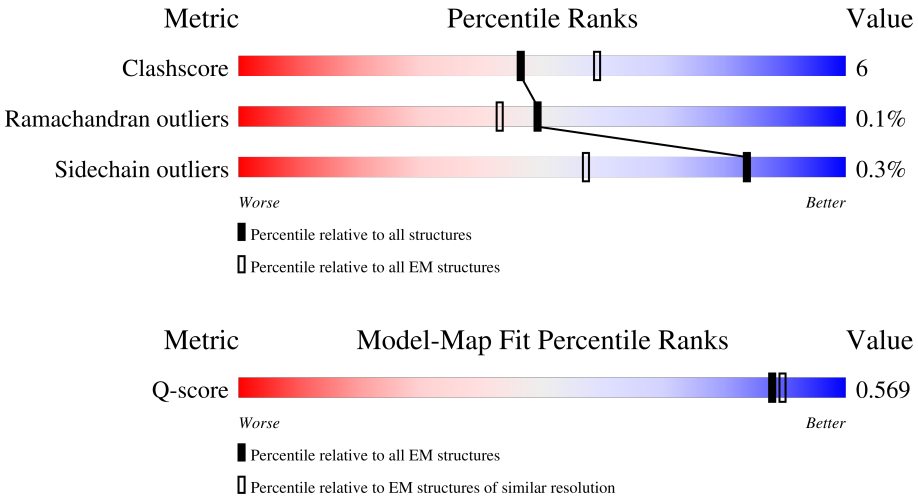
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 <=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	377	85% 13%
1	B	377	86% 12%
1	C	377	20% 82% 16%
2	D	1077	51% 12% 37%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14306 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2893	1833	488	551	21		
1	B	371	Total	C	N	O	S	2	0
			2911	1844	491	555	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

- Molecule 2 is a protein called Unconventional myosin-VIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	681	Total	C	N	O	S	0	0
			5490	3483	955	1018	34		

There are 295 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP P97479
D	-3	ASN	-	expression tag	UNP P97479
D	-2	LYS	-	expression tag	UNP P97479
D	-1	ALA	-	expression tag	UNP P97479
D	0	GLY	-	expression tag	UNP P97479
D	1	MET	-	expression tag	UNP P97479
D	2	GLU	-	expression tag	UNP P97479
D	3	SER	-	expression tag	UNP P97479
D	4	PRO	-	expression tag	UNP P97479
D	5	GLY	-	expression tag	UNP P97479
D	6	SER	-	expression tag	UNP P97479
D	7	PRO	-	expression tag	UNP P97479
D	8	ALA	-	expression tag	UNP P97479
D	9	ASP	-	expression tag	UNP P97479
D	10	PRO	-	expression tag	UNP P97479
D	11	GLY	-	expression tag	UNP P97479
D	12	GLU	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	13	ALA	-	expression tag	UNP P97479
D	14	PRO	-	expression tag	UNP P97479
D	15	ALA	-	expression tag	UNP P97479
D	16	PRO	-	expression tag	UNP P97479
D	17	PRO	-	expression tag	UNP P97479
D	18	PRO	-	expression tag	UNP P97479
D	19	GLY	-	expression tag	UNP P97479
D	20	LYS	-	expression tag	UNP P97479
D	21	TRP	-	expression tag	UNP P97479
D	22	ALA	-	expression tag	UNP P97479
D	23	LEU	-	expression tag	UNP P97479
D	24	VAL	-	expression tag	UNP P97479
D	25	ARG	-	expression tag	UNP P97479
D	26	ASN	-	expression tag	UNP P97479
D	27	LEU	-	expression tag	UNP P97479
D	28	ASN	-	expression tag	UNP P97479
D	29	GLN	-	expression tag	UNP P97479
D	30	THR	-	expression tag	UNP P97479
D	31	LEU	-	expression tag	UNP P97479
D	32	LYS	-	expression tag	UNP P97479
D	33	THR	-	expression tag	UNP P97479
D	34	PHE	-	expression tag	UNP P97479
D	35	ALA	-	expression tag	UNP P97479
D	36	VAL	-	expression tag	UNP P97479
D	37	LEU	-	expression tag	UNP P97479
D	38	PRO	-	expression tag	UNP P97479
D	821	GLY	-	expression tag	UNP P97479
D	822	SER	-	expression tag	UNP P97479
D	823	MET	-	expression tag	UNP P97479
D	824	VAL	-	expression tag	UNP P97479
D	825	SER	-	expression tag	UNP P97479
D	826	LYS	-	expression tag	UNP P97479
D	827	GLY	-	expression tag	UNP P97479
D	828	GLU	-	expression tag	UNP P97479
D	829	GLU	-	expression tag	UNP P97479
D	830	LEU	-	expression tag	UNP P97479
D	831	PHE	-	expression tag	UNP P97479
D	832	THR	-	expression tag	UNP P97479
D	833	GLY	-	expression tag	UNP P97479
D	834	VAL	-	expression tag	UNP P97479
D	835	VAL	-	expression tag	UNP P97479
D	836	PRO	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	837	ILE	-	expression tag	UNP P97479
D	838	LEU	-	expression tag	UNP P97479
D	839	VAL	-	expression tag	UNP P97479
D	840	GLU	-	expression tag	UNP P97479
D	841	LEU	-	expression tag	UNP P97479
D	842	ASP	-	expression tag	UNP P97479
D	843	GLY	-	expression tag	UNP P97479
D	844	ASP	-	expression tag	UNP P97479
D	845	VAL	-	expression tag	UNP P97479
D	846	ASN	-	expression tag	UNP P97479
D	847	GLY	-	expression tag	UNP P97479
D	848	HIS	-	expression tag	UNP P97479
D	849	LYS	-	expression tag	UNP P97479
D	850	PHE	-	expression tag	UNP P97479
D	851	SER	-	expression tag	UNP P97479
D	852	VAL	-	expression tag	UNP P97479
D	853	SER	-	expression tag	UNP P97479
D	854	GLY	-	expression tag	UNP P97479
D	855	GLU	-	expression tag	UNP P97479
D	856	GLY	-	expression tag	UNP P97479
D	857	GLU	-	expression tag	UNP P97479
D	858	GLY	-	expression tag	UNP P97479
D	859	ASP	-	expression tag	UNP P97479
D	860	ALA	-	expression tag	UNP P97479
D	861	THR	-	expression tag	UNP P97479
D	862	TYR	-	expression tag	UNP P97479
D	863	GLY	-	expression tag	UNP P97479
D	864	LYS	-	expression tag	UNP P97479
D	865	LEU	-	expression tag	UNP P97479
D	866	THR	-	expression tag	UNP P97479
D	867	LEU	-	expression tag	UNP P97479
D	868	LYS	-	expression tag	UNP P97479
D	869	PHE	-	expression tag	UNP P97479
D	870	ILE	-	expression tag	UNP P97479
D	871	CYS	-	expression tag	UNP P97479
D	872	THR	-	expression tag	UNP P97479
D	873	THR	-	expression tag	UNP P97479
D	874	GLY	-	expression tag	UNP P97479
D	875	LYS	-	expression tag	UNP P97479
D	876	LEU	-	expression tag	UNP P97479
D	877	PRO	-	expression tag	UNP P97479
D	878	VAL	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	879	PRO	-	expression tag	UNP P97479
D	880	TRP	-	expression tag	UNP P97479
D	881	PRO	-	expression tag	UNP P97479
D	882	THR	-	expression tag	UNP P97479
D	883	LEU	-	expression tag	UNP P97479
D	884	VAL	-	expression tag	UNP P97479
D	885	THR	-	expression tag	UNP P97479
D	886	THR	-	expression tag	UNP P97479
D	887	LEU	-	expression tag	UNP P97479
D	888	THR	-	expression tag	UNP P97479
D	889	TYR	-	expression tag	UNP P97479
D	890	GLY	-	expression tag	UNP P97479
D	891	VAL	-	expression tag	UNP P97479
D	892	GLN	-	expression tag	UNP P97479
D	893	CYS	-	expression tag	UNP P97479
D	894	PHE	-	expression tag	UNP P97479
D	895	SER	-	expression tag	UNP P97479
D	896	ARG	-	expression tag	UNP P97479
D	897	TYR	-	expression tag	UNP P97479
D	898	PRO	-	expression tag	UNP P97479
D	899	ASP	-	expression tag	UNP P97479
D	900	HIS	-	expression tag	UNP P97479
D	901	MET	-	expression tag	UNP P97479
D	902	LYS	-	expression tag	UNP P97479
D	903	GLN	-	expression tag	UNP P97479
D	904	HIS	-	expression tag	UNP P97479
D	905	ASP	-	expression tag	UNP P97479
D	906	PHE	-	expression tag	UNP P97479
D	907	PHE	-	expression tag	UNP P97479
D	908	LYS	-	expression tag	UNP P97479
D	909	SER	-	expression tag	UNP P97479
D	910	ALA	-	expression tag	UNP P97479
D	911	MET	-	expression tag	UNP P97479
D	912	PRO	-	expression tag	UNP P97479
D	913	GLU	-	expression tag	UNP P97479
D	914	GLY	-	expression tag	UNP P97479
D	915	TYR	-	expression tag	UNP P97479
D	916	VAL	-	expression tag	UNP P97479
D	917	GLN	-	expression tag	UNP P97479
D	918	GLU	-	expression tag	UNP P97479
D	919	ARG	-	expression tag	UNP P97479
D	920	THR	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	921	ILE	-	expression tag	UNP P97479
D	922	PHE	-	expression tag	UNP P97479
D	923	PHE	-	expression tag	UNP P97479
D	924	LYS	-	expression tag	UNP P97479
D	925	ASP	-	expression tag	UNP P97479
D	926	ASP	-	expression tag	UNP P97479
D	927	GLY	-	expression tag	UNP P97479
D	928	ASN	-	expression tag	UNP P97479
D	929	TYR	-	expression tag	UNP P97479
D	930	LYS	-	expression tag	UNP P97479
D	931	THR	-	expression tag	UNP P97479
D	932	ARG	-	expression tag	UNP P97479
D	933	ALA	-	expression tag	UNP P97479
D	934	GLU	-	expression tag	UNP P97479
D	935	VAL	-	expression tag	UNP P97479
D	936	LYS	-	expression tag	UNP P97479
D	937	PHE	-	expression tag	UNP P97479
D	938	GLU	-	expression tag	UNP P97479
D	939	GLY	-	expression tag	UNP P97479
D	940	ASP	-	expression tag	UNP P97479
D	941	THR	-	expression tag	UNP P97479
D	942	LEU	-	expression tag	UNP P97479
D	943	VAL	-	expression tag	UNP P97479
D	944	ASN	-	expression tag	UNP P97479
D	945	ARG	-	expression tag	UNP P97479
D	946	ILE	-	expression tag	UNP P97479
D	947	GLU	-	expression tag	UNP P97479
D	948	LEU	-	expression tag	UNP P97479
D	949	LYS	-	expression tag	UNP P97479
D	950	GLY	-	expression tag	UNP P97479
D	951	ILE	-	expression tag	UNP P97479
D	952	ASP	-	expression tag	UNP P97479
D	953	PHE	-	expression tag	UNP P97479
D	954	LYS	-	expression tag	UNP P97479
D	955	GLU	-	expression tag	UNP P97479
D	956	ASP	-	expression tag	UNP P97479
D	957	GLY	-	expression tag	UNP P97479
D	958	ASN	-	expression tag	UNP P97479
D	959	ILE	-	expression tag	UNP P97479
D	960	LEU	-	expression tag	UNP P97479
D	961	GLY	-	expression tag	UNP P97479
D	962	HIS	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	963	LYS	-	expression tag	UNP P97479
D	964	LEU	-	expression tag	UNP P97479
D	965	GLU	-	expression tag	UNP P97479
D	966	TYR	-	expression tag	UNP P97479
D	967	ASN	-	expression tag	UNP P97479
D	968	TYR	-	expression tag	UNP P97479
D	969	ASN	-	expression tag	UNP P97479
D	970	SER	-	expression tag	UNP P97479
D	971	HIS	-	expression tag	UNP P97479
D	972	ASN	-	expression tag	UNP P97479
D	973	VAL	-	expression tag	UNP P97479
D	974	TYR	-	expression tag	UNP P97479
D	975	ILE	-	expression tag	UNP P97479
D	976	MET	-	expression tag	UNP P97479
D	977	ALA	-	expression tag	UNP P97479
D	978	ASP	-	expression tag	UNP P97479
D	979	LYS	-	expression tag	UNP P97479
D	980	GLN	-	expression tag	UNP P97479
D	981	LYS	-	expression tag	UNP P97479
D	982	ASN	-	expression tag	UNP P97479
D	983	GLY	-	expression tag	UNP P97479
D	984	ILE	-	expression tag	UNP P97479
D	985	LYS	-	expression tag	UNP P97479
D	986	VAL	-	expression tag	UNP P97479
D	987	ASN	-	expression tag	UNP P97479
D	988	PHE	-	expression tag	UNP P97479
D	989	LYS	-	expression tag	UNP P97479
D	990	ILE	-	expression tag	UNP P97479
D	991	ARG	-	expression tag	UNP P97479
D	992	HIS	-	expression tag	UNP P97479
D	993	ASN	-	expression tag	UNP P97479
D	994	ILE	-	expression tag	UNP P97479
D	995	GLU	-	expression tag	UNP P97479
D	996	ASP	-	expression tag	UNP P97479
D	997	GLY	-	expression tag	UNP P97479
D	998	SER	-	expression tag	UNP P97479
D	999	VAL	-	expression tag	UNP P97479
D	1000	GLN	-	expression tag	UNP P97479
D	1001	LEU	-	expression tag	UNP P97479
D	1002	ALA	-	expression tag	UNP P97479
D	1003	ASP	-	expression tag	UNP P97479
D	1004	HIS	-	expression tag	UNP P97479

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1005	TYR	-	expression tag	UNP P97479
D	1006	GLN	-	expression tag	UNP P97479
D	1007	GLN	-	expression tag	UNP P97479
D	1008	ASN	-	expression tag	UNP P97479
D	1009	THR	-	expression tag	UNP P97479
D	1010	PRO	-	expression tag	UNP P97479
D	1011	ILE	-	expression tag	UNP P97479
D	1012	GLY	-	expression tag	UNP P97479
D	1013	ASP	-	expression tag	UNP P97479
D	1014	GLY	-	expression tag	UNP P97479
D	1015	PRO	-	expression tag	UNP P97479
D	1016	VAL	-	expression tag	UNP P97479
D	1017	LEU	-	expression tag	UNP P97479
D	1018	LEU	-	expression tag	UNP P97479
D	1019	PRO	-	expression tag	UNP P97479
D	1020	ASP	-	expression tag	UNP P97479
D	1021	ASN	-	expression tag	UNP P97479
D	1022	HIS	-	expression tag	UNP P97479
D	1023	TYR	-	expression tag	UNP P97479
D	1024	LEU	-	expression tag	UNP P97479
D	1025	SER	-	expression tag	UNP P97479
D	1026	THR	-	expression tag	UNP P97479
D	1027	GLN	-	expression tag	UNP P97479
D	1028	SER	-	expression tag	UNP P97479
D	1029	ALA	-	expression tag	UNP P97479
D	1030	LEU	-	expression tag	UNP P97479
D	1031	SER	-	expression tag	UNP P97479
D	1032	LYS	-	expression tag	UNP P97479
D	1033	ASP	-	expression tag	UNP P97479
D	1034	PRO	-	expression tag	UNP P97479
D	1035	ASN	-	expression tag	UNP P97479
D	1036	GLU	-	expression tag	UNP P97479
D	1037	LYS	-	expression tag	UNP P97479
D	1038	ARG	-	expression tag	UNP P97479
D	1039	ASP	-	expression tag	UNP P97479
D	1040	HIS	-	expression tag	UNP P97479
D	1041	MET	-	expression tag	UNP P97479
D	1042	VAL	-	expression tag	UNP P97479
D	1043	LEU	-	expression tag	UNP P97479
D	1044	LEU	-	expression tag	UNP P97479
D	1045	GLU	-	expression tag	UNP P97479
D	1046	PHE	-	expression tag	UNP P97479

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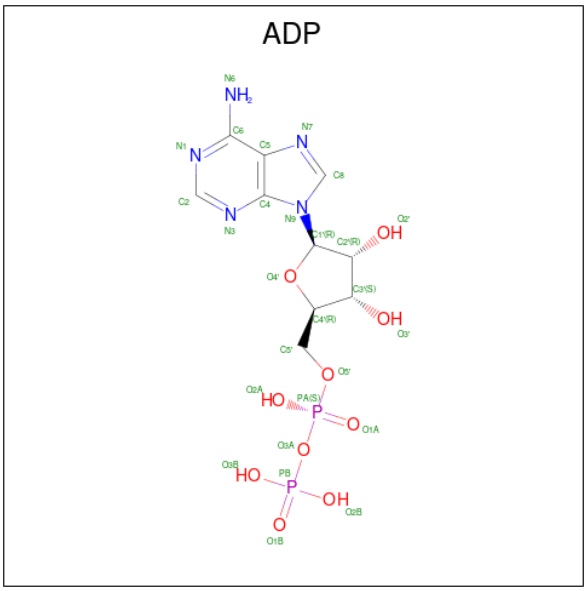
Chain	Residue	Modelled	Actual	Comment	Reference
D	1047	VAL	-	expression tag	UNP P97479
D	1048	THR	-	expression tag	UNP P97479
D	1049	ALA	-	expression tag	UNP P97479
D	1050	ALA	-	expression tag	UNP P97479
D	1051	GLY	-	expression tag	UNP P97479
D	1052	ILE	-	expression tag	UNP P97479
D	1053	THR	-	expression tag	UNP P97479
D	1054	LEU	-	expression tag	UNP P97479
D	1055	GLY	-	expression tag	UNP P97479
D	1056	MET	-	expression tag	UNP P97479
D	1057	ASP	-	expression tag	UNP P97479
D	1058	GLU	-	expression tag	UNP P97479
D	1059	LEU	-	expression tag	UNP P97479
D	1060	TYR	-	expression tag	UNP P97479
D	1061	LYS	-	expression tag	UNP P97479
D	1062	ALA	-	expression tag	UNP P97479
D	1063	ALA	-	expression tag	UNP P97479
D	1064	ALA	-	expression tag	UNP P97479
D	1065	ASP	-	expression tag	UNP P97479
D	1066	TYR	-	expression tag	UNP P97479
D	1067	LYS	-	expression tag	UNP P97479
D	1068	ASP	-	expression tag	UNP P97479
D	1069	ASP	-	expression tag	UNP P97479
D	1070	ASP	-	expression tag	UNP P97479
D	1071	ASP	-	expression tag	UNP P97479
D	1072	LYS	-	expression tag	UNP P97479

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

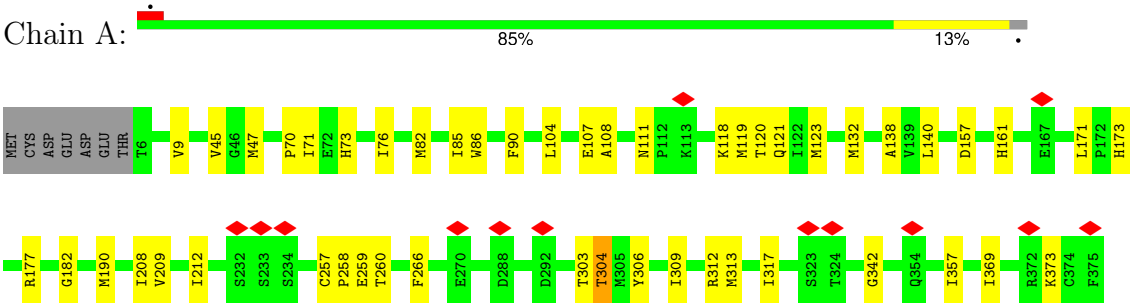
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

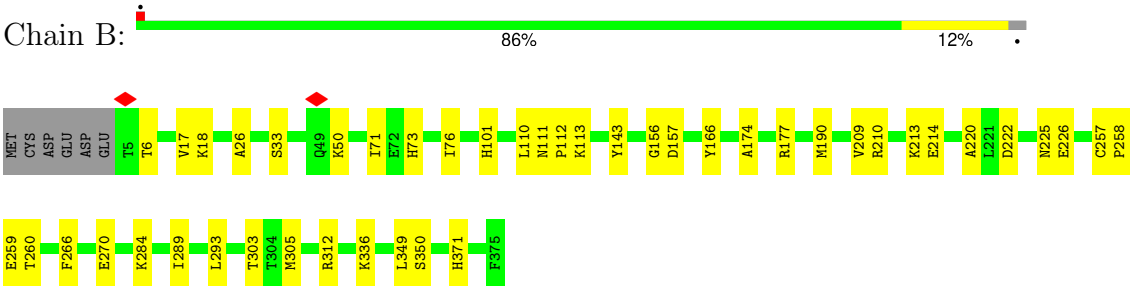
• Molecule 1: Actin, alpha skeletal muscle

Chain A:



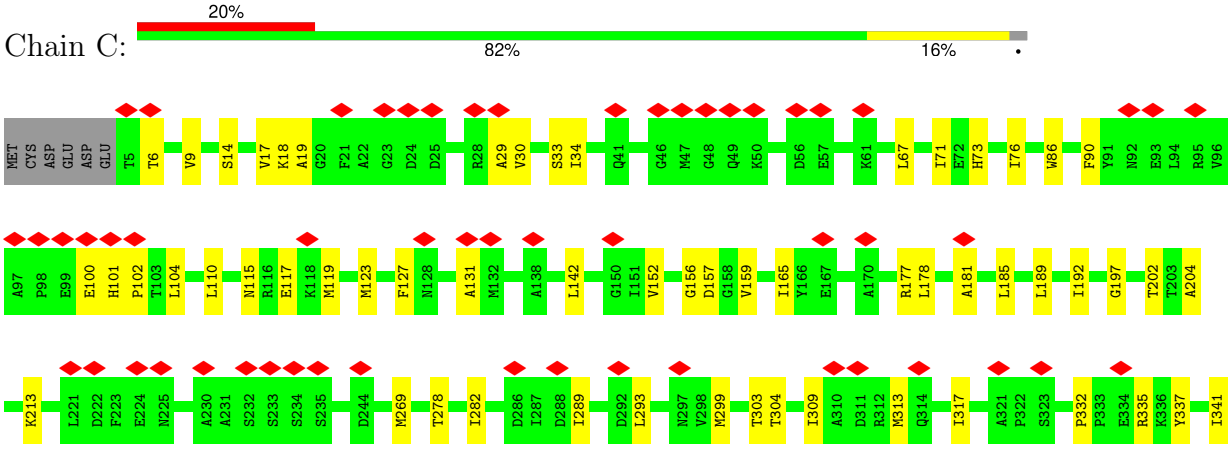
• Molecule 1: Actin, alpha skeletal muscle

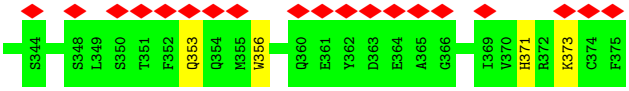
Chain B:



• Molecule 1: Actin, alpha skeletal muscle

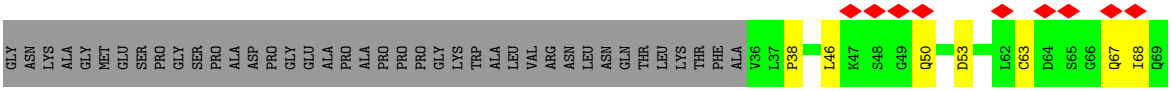
Chain C:

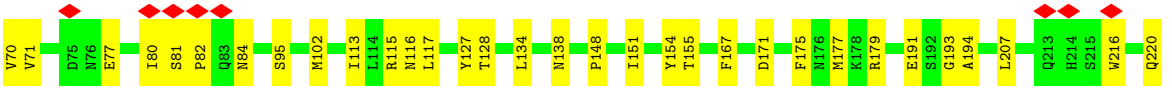


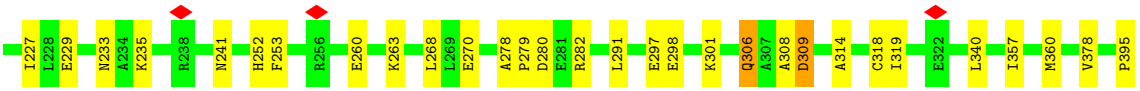


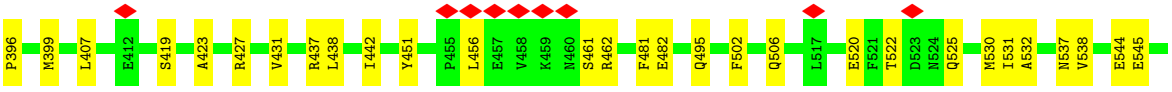
• Molecule 2: Unconventional myosin-VIIa

Chain D:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0.0°, rise=0.001 Å, axial sym=C1	Depositor
Number of segments used	878646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.199	Depositor
Minimum map value	-2.498	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	552.96, 552.96, 552.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HIC, ADP

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	0.18	0/2943	0.36	1/3984 (0.0%)
1	B	0.14	0/2961	0.35	0/4009
1	C	0.18	0/2950	0.34	0/3994
2	D	0.19	0/5610	0.38	1/7581 (0.0%)
All	All	0.18	0/14464	0.36	2/19568 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	THR	N-CA-C	-5.26	106.45	112.92
2	D	308	ALA	N-CA-C	-5.01	106.86	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2893	0	2865	31	0
1	B	2911	0	2883	33	0
1	C	2900	0	2872	36	0
2	D	5490	0	5419	80	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	4	0
3	C	27	0	12	2	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	14306	0	14087	172	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 172 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)
2:D:252:HIS:HB3	2:D:462:ARG:HD2	1.61	0.81
1:C:178:LEU:HD11	1:C:269:MET:HE1	1.66	0.76
2:D:280:ASP:HA	2:D:318:CYS:SG	2.28	0.73
1:C:202:THR:HG22	1:C:204:ALA:H	1.53	0.73
1:B:222:ASP:OD2	1:B:225:ASN:ND2	2.25	0.70

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	367/377 (97%)	360 (98%)	7 (2%)	0	100	100
1	B	370/377 (98%)	361 (98%)	9 (2%)	0	100	100
1	C	368/377 (98%)	361 (98%)	7 (2%)	0	100	100
2	D	679/1077 (63%)	651 (96%)	27 (4%)	1 (0%)	48	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1784/2208 (81%)	1733 (97%)	50 (3%)	1 (0%)	49 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	306	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	312/319 (98%)	312 (100%)	0	100 100
1	B	314/319 (98%)	314 (100%)	0	100 100
1	C	313/319 (98%)	311 (99%)	2 (1%)	78 83
2	D	602/940 (64%)	600 (100%)	2 (0%)	86 87
All	All	1541/1897 (81%)	1537 (100%)	4 (0%)	84 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	152	VAL
1	C	159	VAL
2	D	268	LEU
2	D	309	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	311	ASN
2	D	490	ASN
2	D	687	GLN
2	D	595	GLN
2	D	682	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HIC	B	73	1	10,11,12	1.49	1 (10%)	9,14,16	1.22	1 (11%)
1	HIC	C	73	1	10,11,12	1.53	1 (10%)	9,14,16	1.23	1 (11%)
1	HIC	A	73	1	10,11,12	1.52	1 (10%)	9,14,16	1.23	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	B	73	1	-	0/5/6/8	0/1/1/1
1	HIC	C	73	1	-	0/5/6/8	0/1/1/1
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	3.08	1.41	1.36
1	C	73	HIC	CD2-CG	3.07	1.41	1.36
1	B	73	HIC	CD2-CG	2.96	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	HIC	NE2-CE1-ND1	-3.00	111.52	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	HIC	NE2-CE1-ND1	-2.94	111.54	112.66
1	C	73	HIC	NE2-CE1-ND1	-2.92	111.55	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ADP	A	401	4	28,29,29	1.42	5 (17%)	43,45,45	1.82	9 (20%)
3	ADP	C	401	4	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
3	ADP	D	1102	4	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	B	401	4	28,29,29	1.41	5 (17%)	43,45,45	1.81	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	401	4	-	7/16/32/32	0/3/3/3
3	ADP	C	401	4	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1102	4	-	0/16/32/32	0/3/3/3
3	ADP	B	401	4	-	5/16/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	ADP	C5-C4	4.69	1.47	1.39
3	A	401	ADP	C5-C4	4.67	1.47	1.39
3	C	401	ADP	C5-C4	4.65	1.47	1.39
3	B	401	ADP	C5-C4	4.59	1.47	1.39
3	C	401	ADP	C5-C6	2.72	1.48	1.41

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ADP	C5-C4-N3	-5.95	118.52	126.72
3	D	1102	ADP	C5-C4-N3	-5.84	118.67	126.72
3	C	401	ADP	C5-C4-N3	-5.81	118.72	126.72
3	B	401	ADP	C5-C4-N3	-5.75	118.80	126.72
3	A	401	ADP	N3-C4-N9	4.63	135.03	127.17

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	C5'-O5'-PA-O1A
3	A	401	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

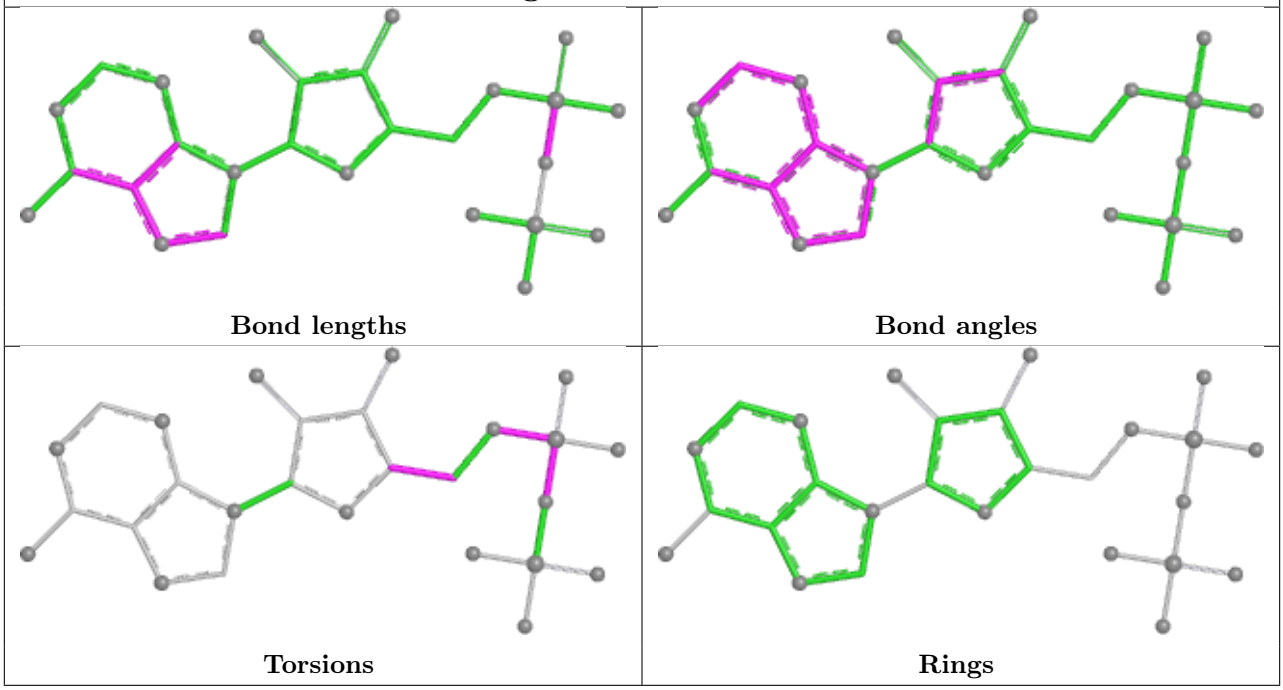
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ADP	2	0
3	B	401	ADP	4	0

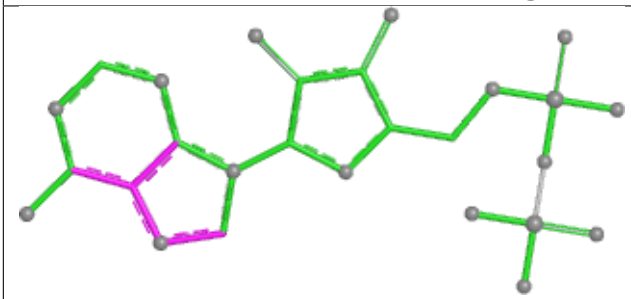
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

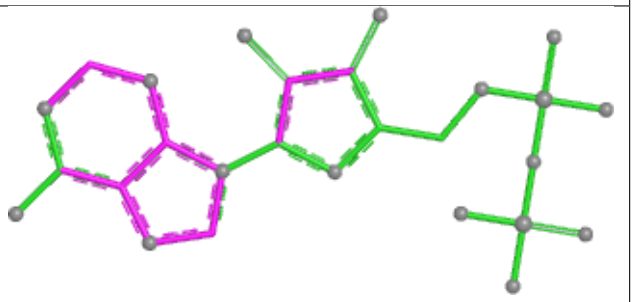
Ligand ADP A 401



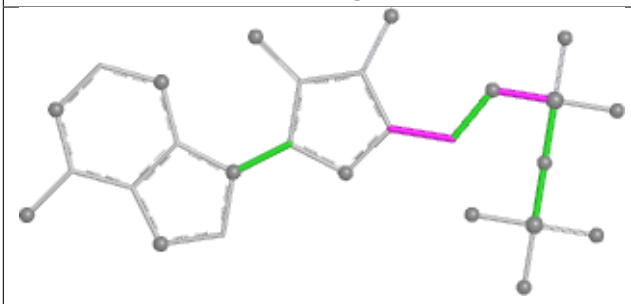
Ligand ADP C 401



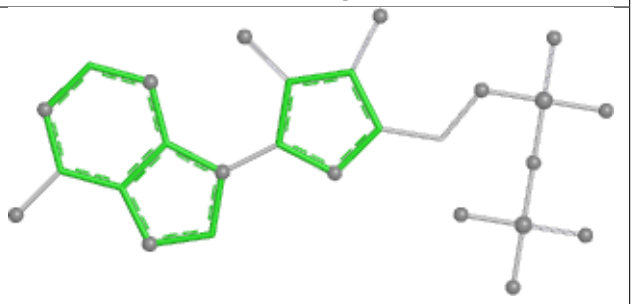
Bond lengths



Bond angles

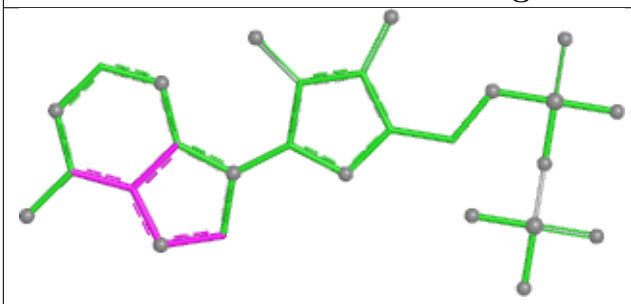


Torsions

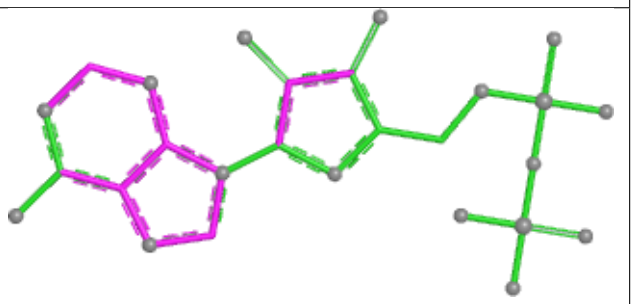


Rings

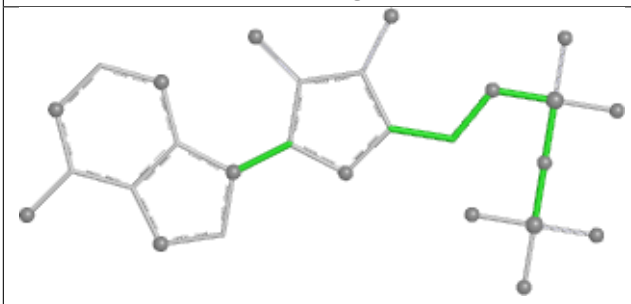
Ligand ADP D 1102



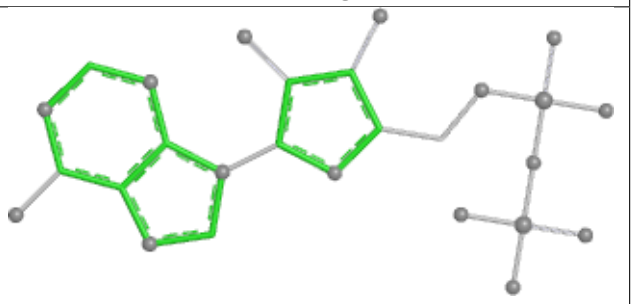
Bond lengths



Bond angles

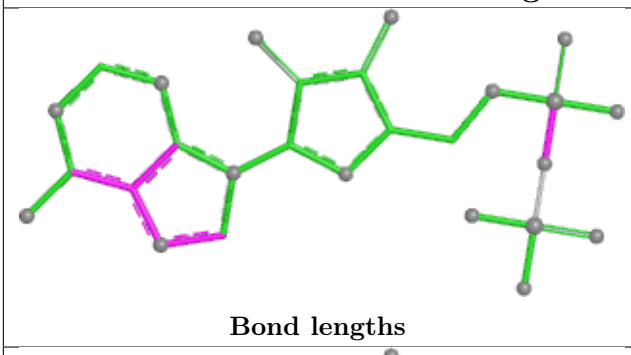


Torsions

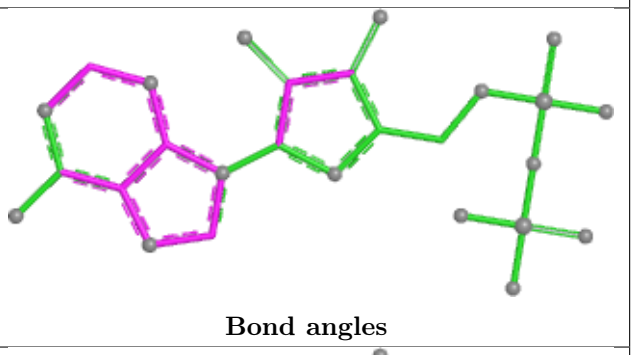


Rings

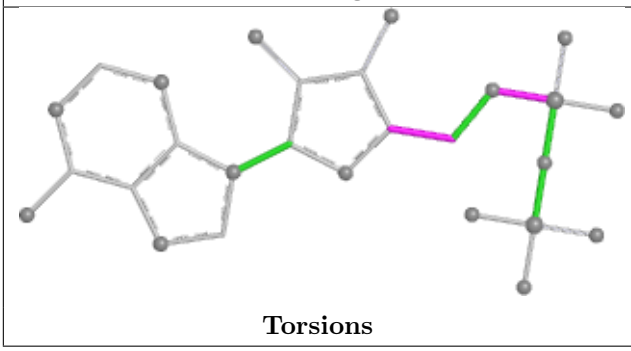
Ligand ADP B 401



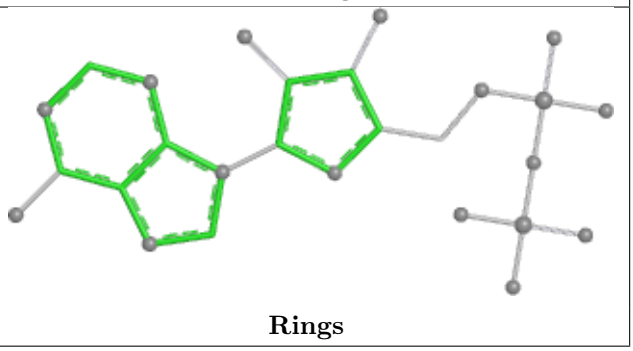
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

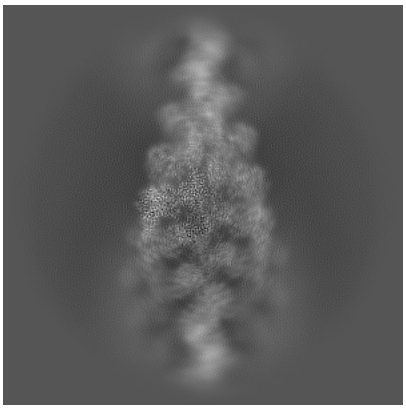
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46818. These allow visual inspection of the internal detail of the map and identification of artifacts.

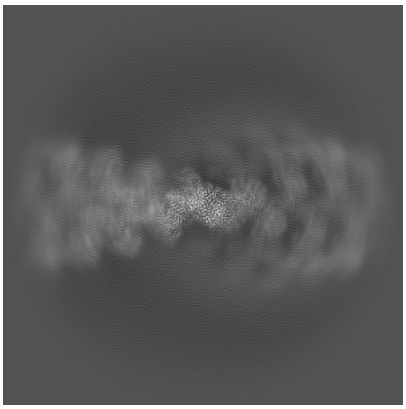
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

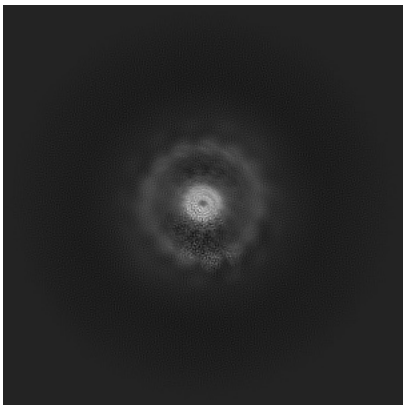
6.1.1 Primary map



X

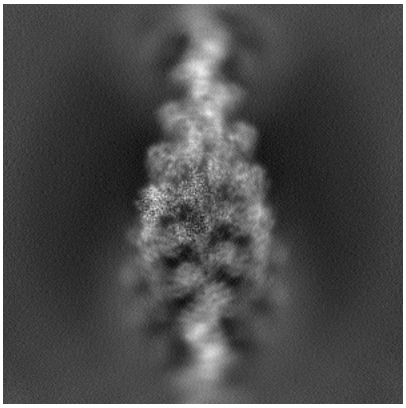


Y

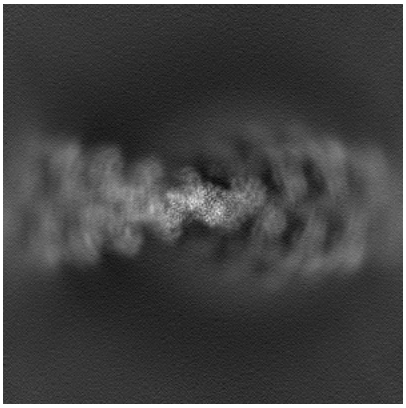


Z

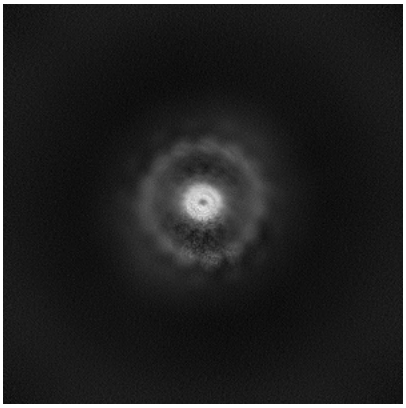
6.1.2 Raw map



X



Y

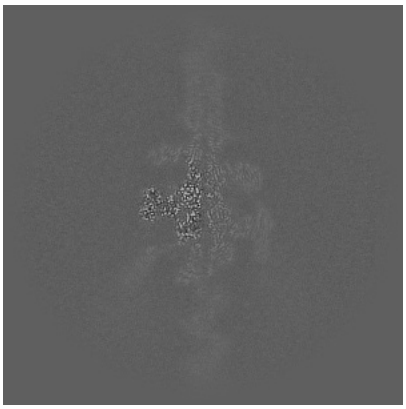


Z

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

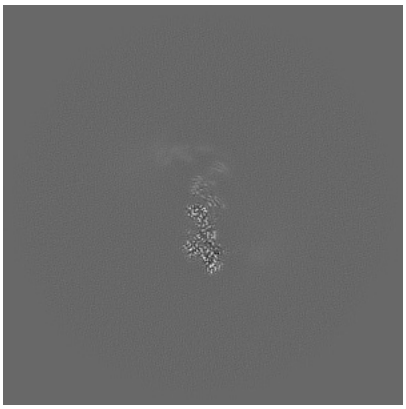
6.2 Central slices (i)

6.2.1 Primary map



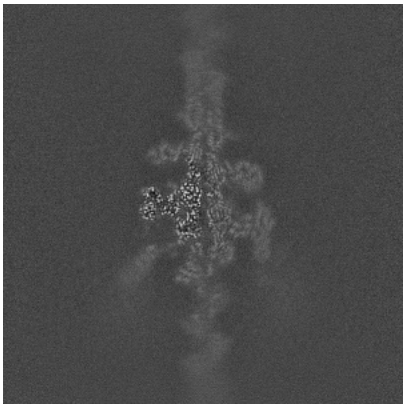
X Index: 256

Y Index: 256

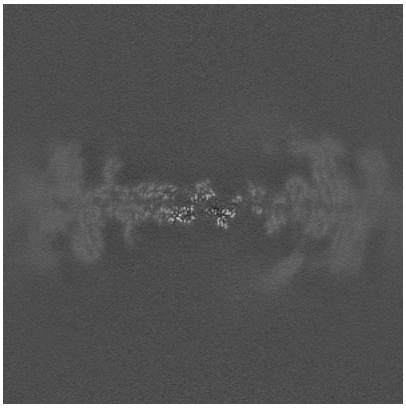


Z Index: 256

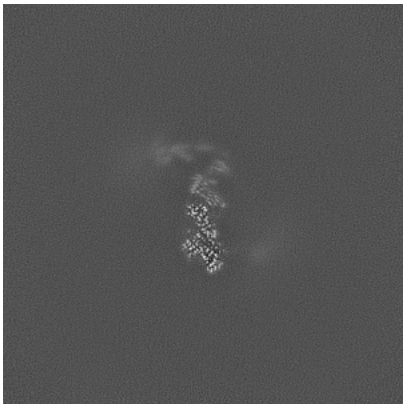
6.2.2 Raw map



X Index: 256



Y Index: 256

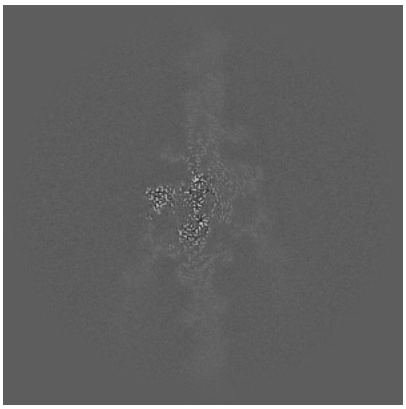


Z Index: 256

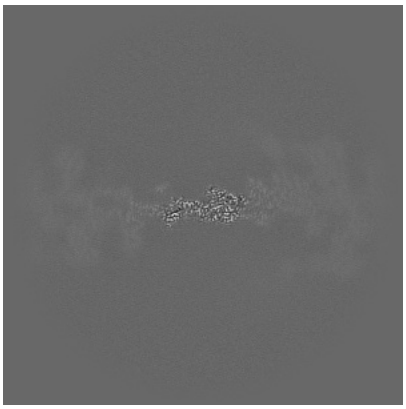
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

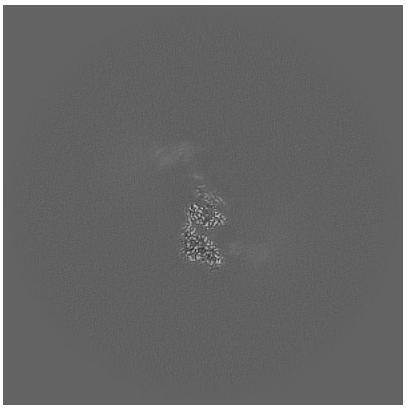
6.3.1 Primary map



X Index: 248

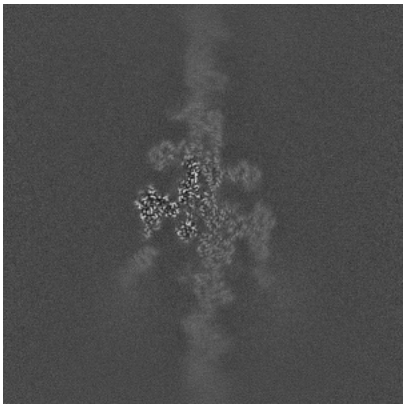


Y Index: 245

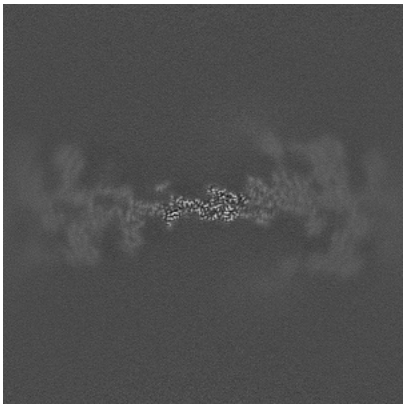


Z Index: 263

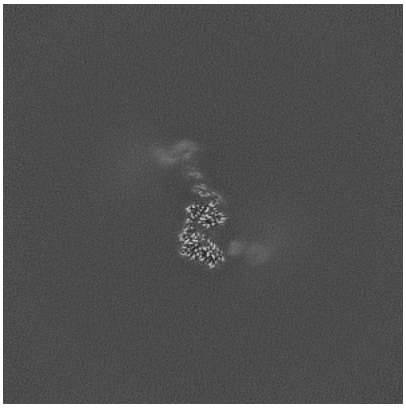
6.3.2 Raw map



X Index: 262



Y Index: 245

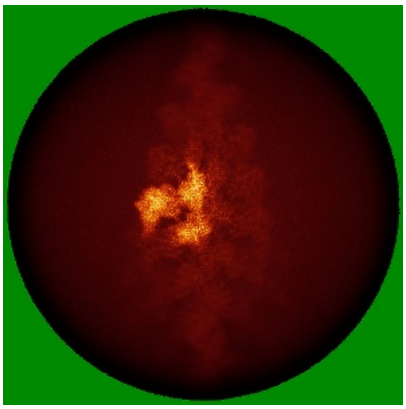


Z Index: 265

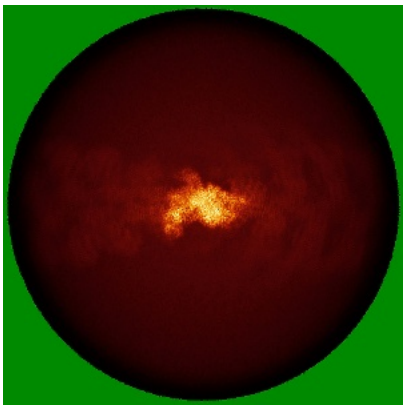
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

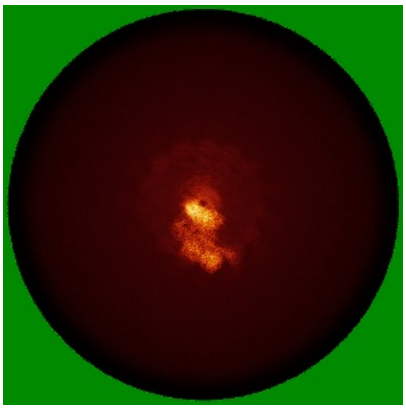
6.4.1 Primary map



X

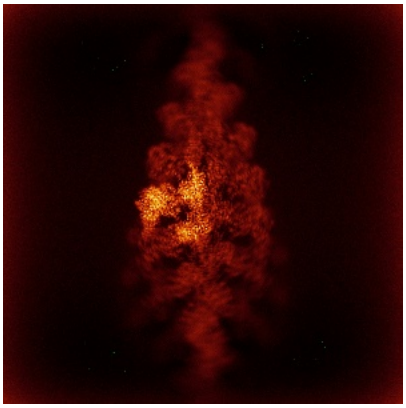


Y

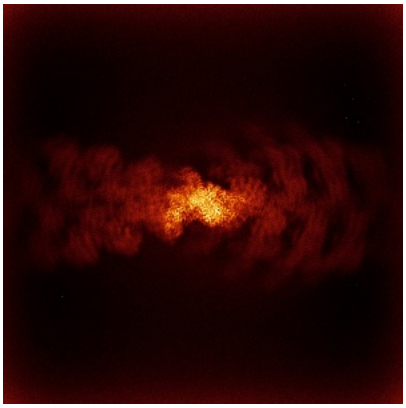


Z

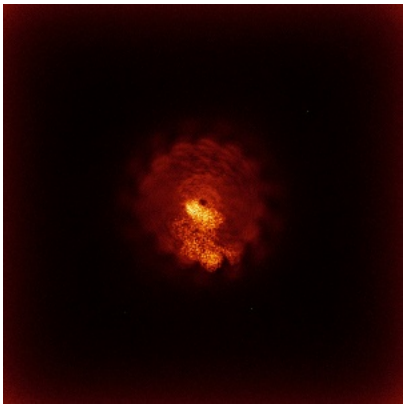
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.32. 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

X Y Z

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.

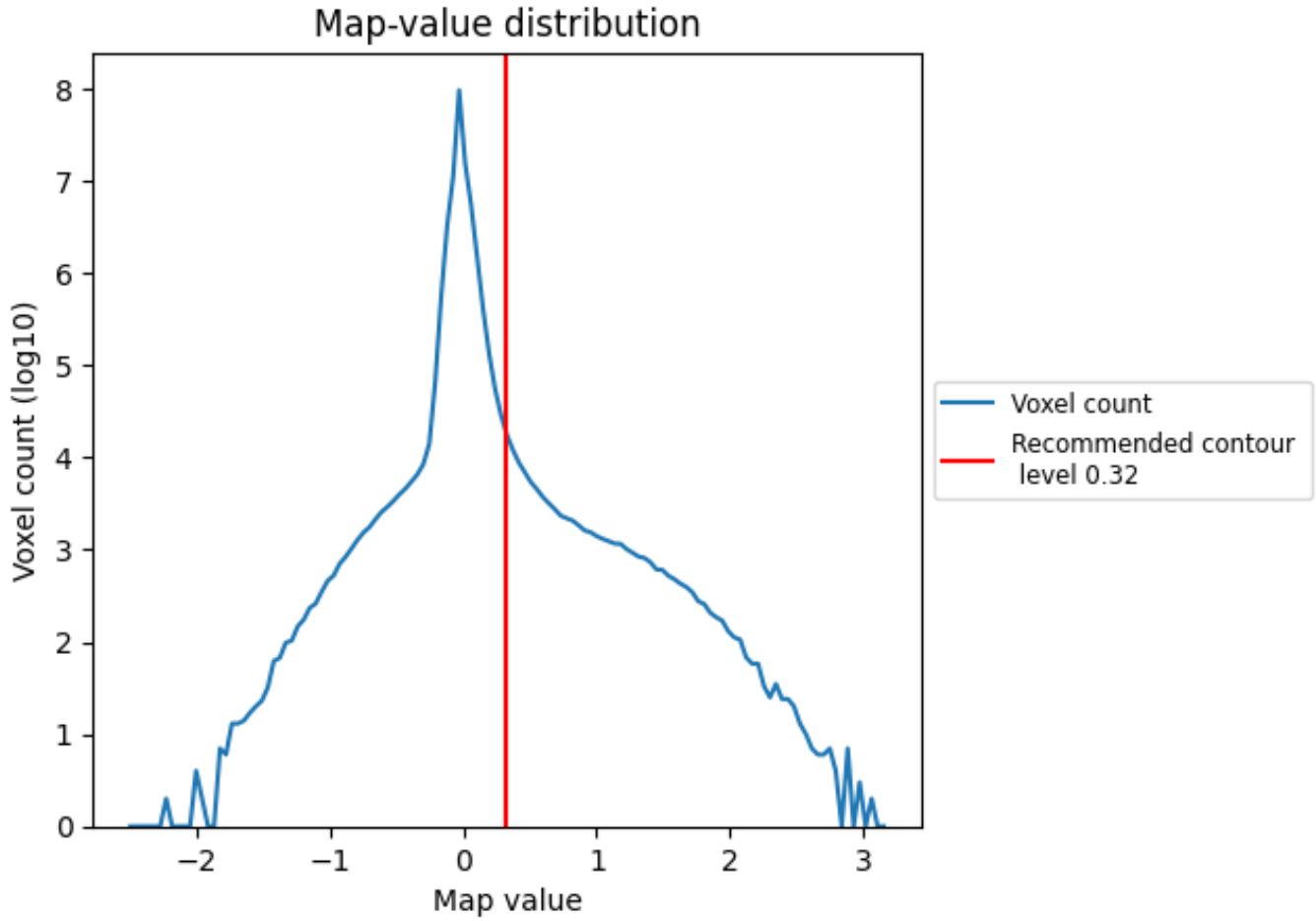
6.6 Mask visualisation (i)

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

7 Map analysis

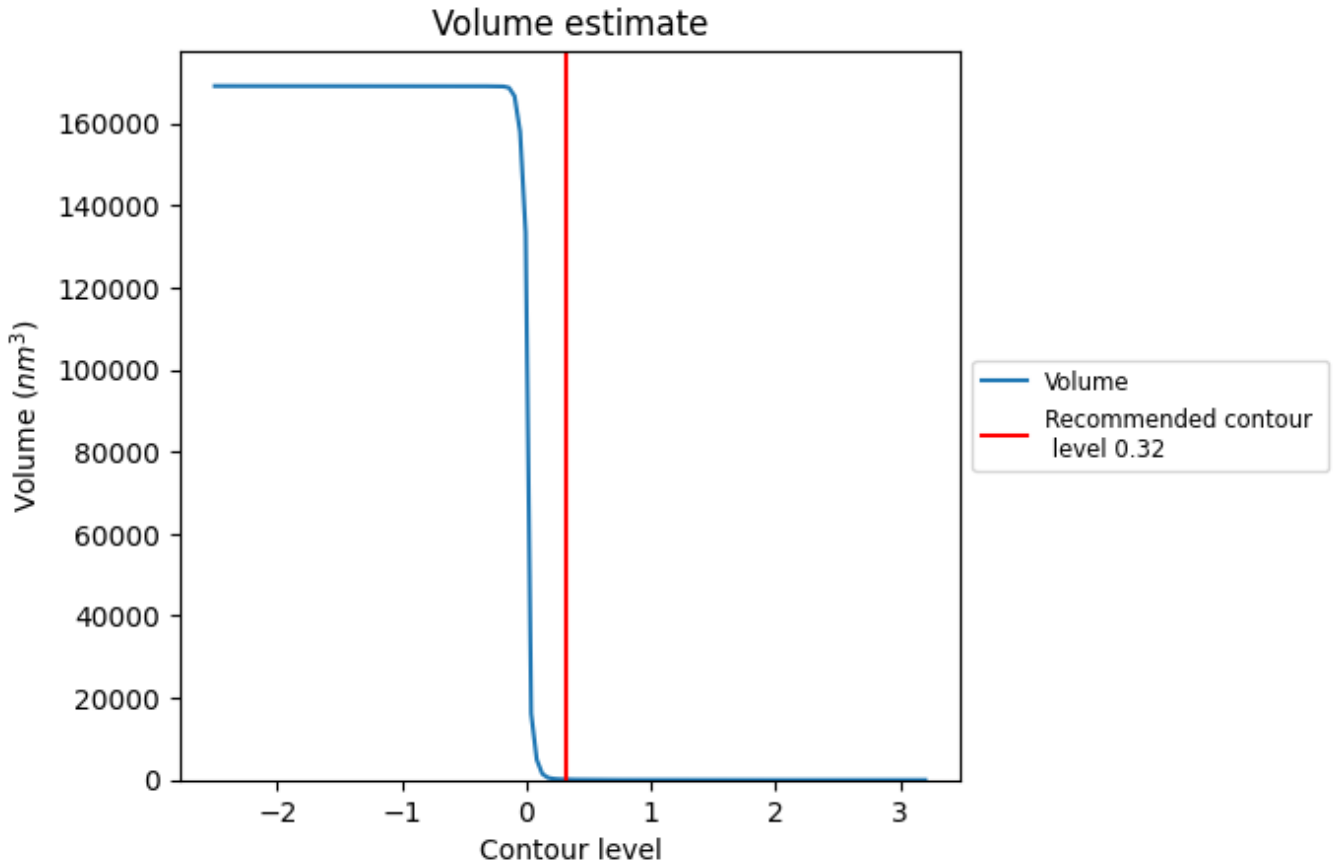
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

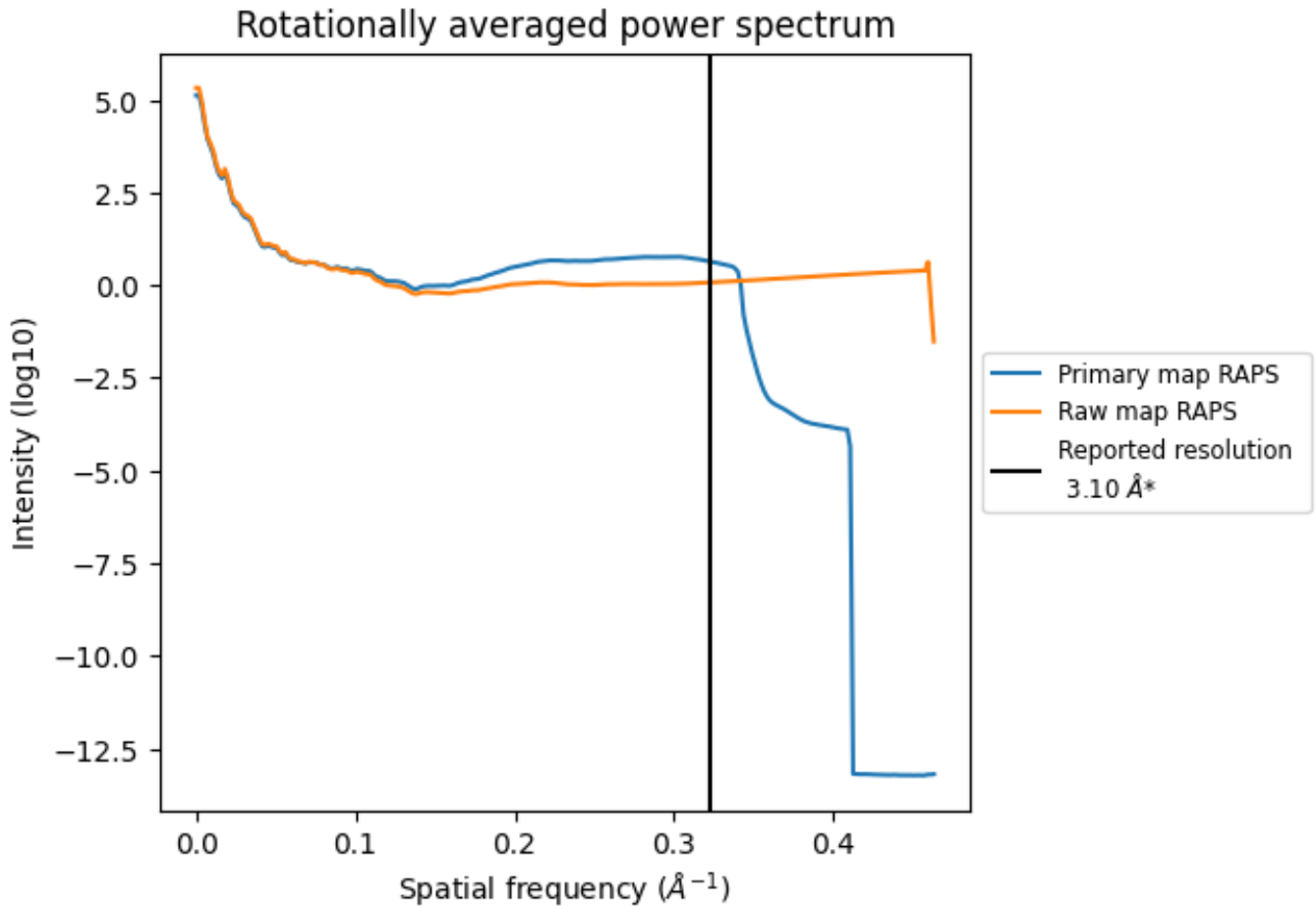
7.2 Volume estimate (i)



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 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 (i)

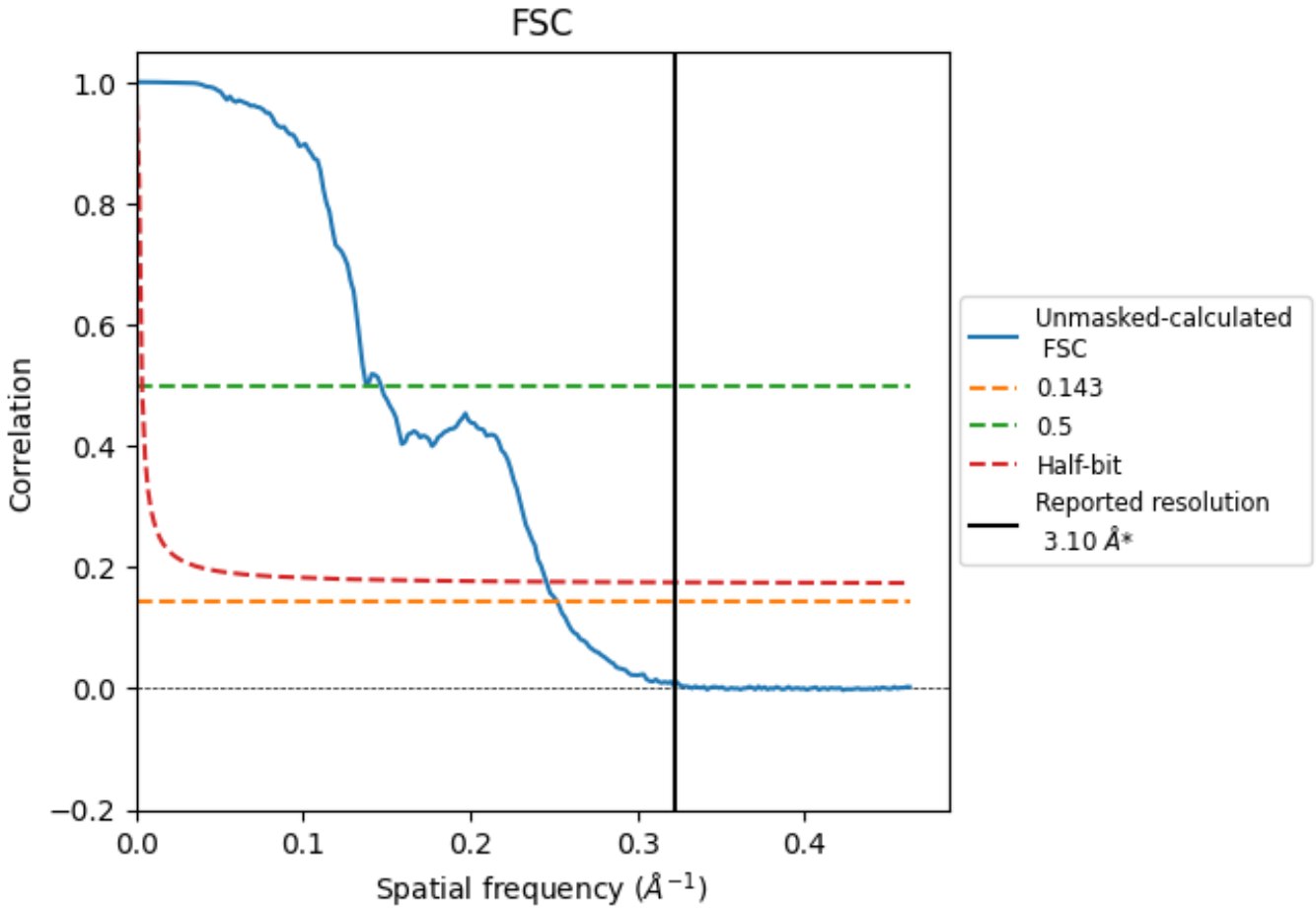


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

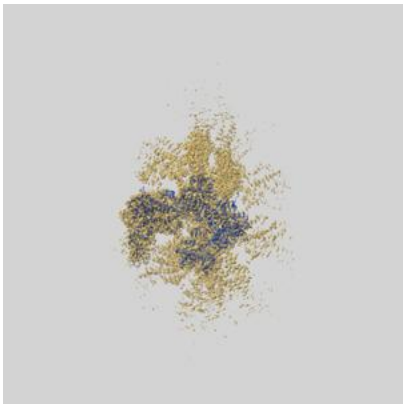
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	6.83	4.07

*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 3.97 differs from the reported value 3.1 by more than 10 %

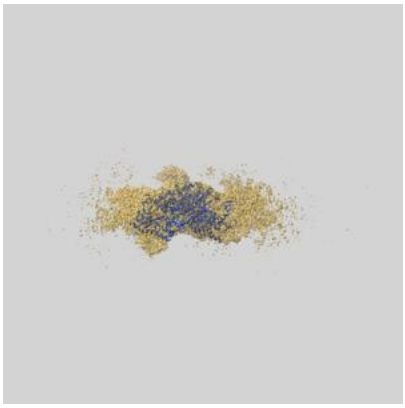
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46818 and PDB model 9DFS. Per-residue inclusion information can be found in section 3 on page 12.

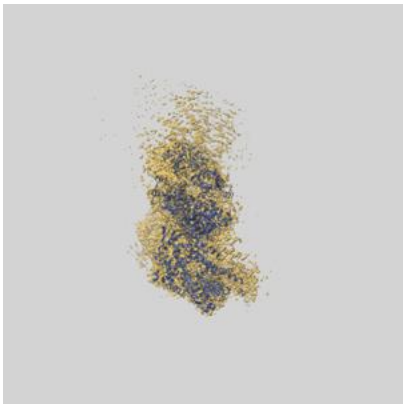
9.1 Map-model overlay



X



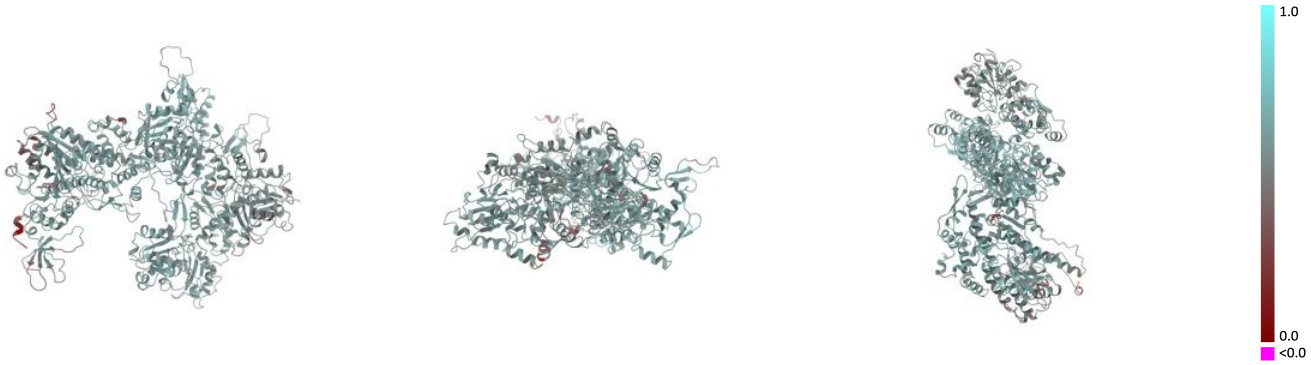
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.32 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.

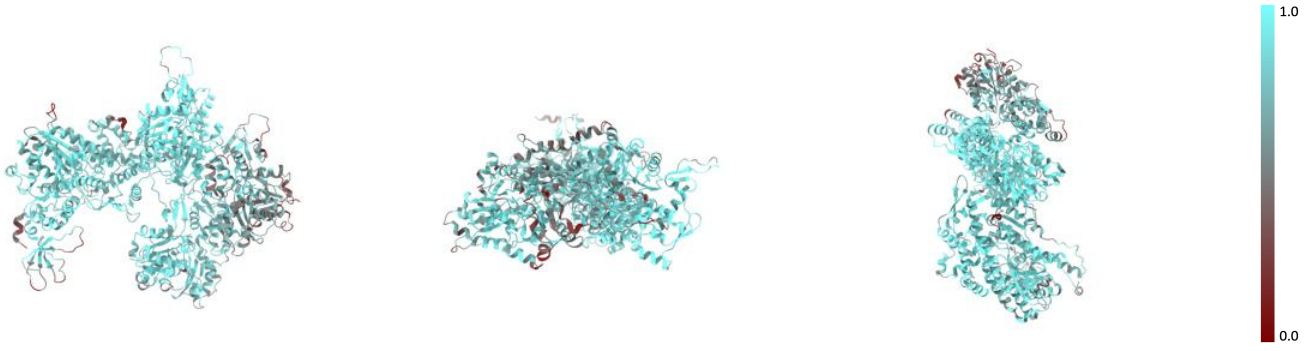
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

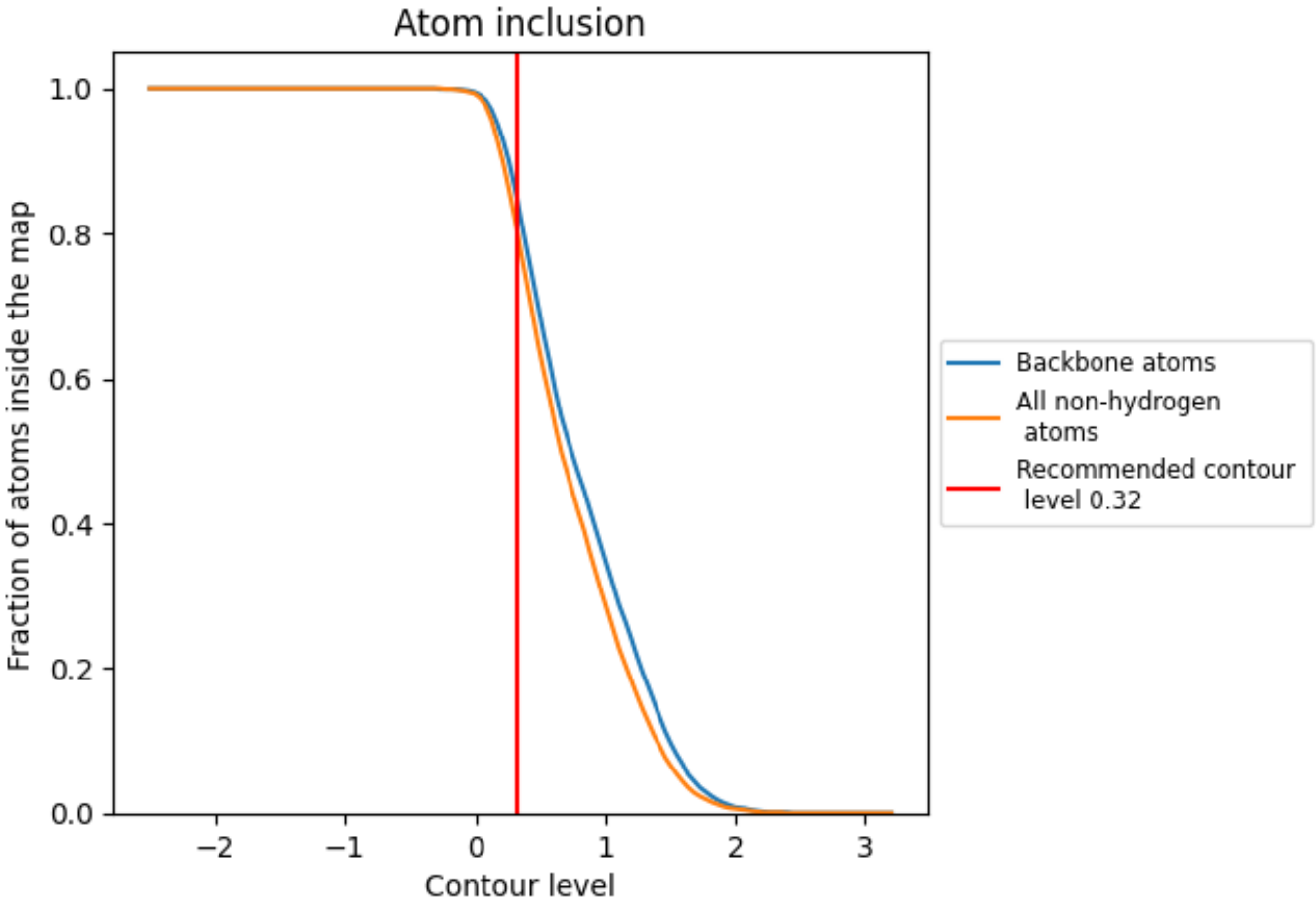
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.32).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.5690
A	0.8460	0.5890
B	0.9210	0.6040
C	0.6150	0.5390
D	0.8290	0.5550